Supporting Information

Copper(II)-Catalyzed Synthesis of Sulfonyl-functionalized Quinone-fused Cyclopenta[*b*]indoles via Four-component Cascade Annulation

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Contents

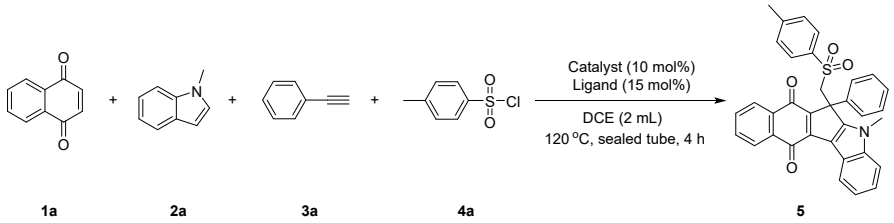
1.General Information

Unless otherwise noted, all reagents were from commercial sources and used as received without further purification. Column chromatography was generally performed on silica gel (200-300 mesh) and reactions were monitored by thin layer chromatography (GF-254 silica gel plate) using UV light (254 nm) to visualize the course of the reactions. ^{1}H, ^{13}C NMR spectra were recorded spectra were recorded at 400 MHz on an Agilent spectrometer. Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated s (singlet), d (doublet), t (triplet), dd (doublet of doublets), m (multiplet); coupling constants (*J*) are in Hertz (Hz). NMR spectra were taken using TMS (1H, δ = 0), $CDCl_3$ (^{1}H, δ = 7.26), and $CDCl_3$ (^{13}C, CPD δ = 77.16) as the internal standards, respectively. HRMS were undertaken on a Thermo Scientific LTQ Orbitrap XL instrument. Melting points were tested with Hanon MP430.

2. Methods and Experimental Procedures

2.1Tables for the optimization of reaction conditions

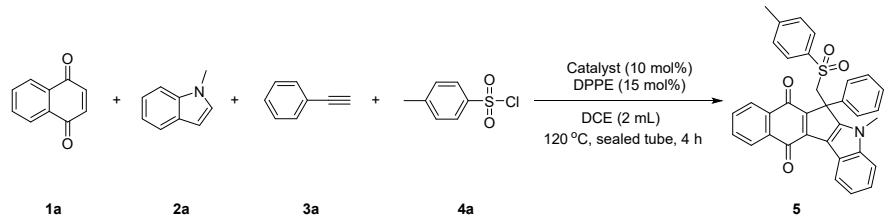
Table S1 Screening of the necessity of catalyst and ligand [a, b, c]



Entry	Catalyst	Ligand	Yield (%)
1	$Cu(acac)_2$	DPPE	49
2	$Cu(acac)_2$	-	35
3	-	DPPE	N.D
4	-	-	N.D

Reaction conditions: [a] **1a** (0.2 mmol), **2a** (0.2 mmol), **3a** (0.6 mmol)，**4a** (0.6 mmol)，catalyst (10 mol%), ligand (15 mol%), DCE (2 mL), T =120 °C, t=4 h. [b] Isolated yield. [c] N.D means not detected.

Table S2 Screening of catalyst [a, b, c]

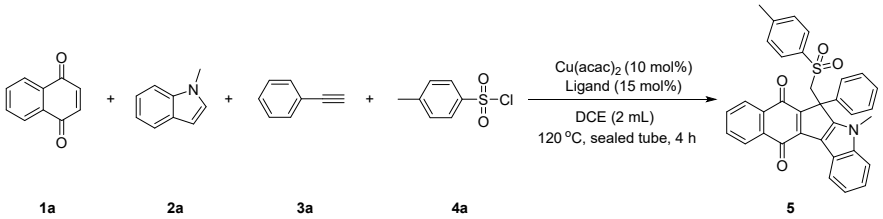


Entry	Catalyst	Yield (%)
1	$Cu(acac)_2$	49
2	$Cu(OTf)_2$	41
3	$Cu(OAc)_2$	32
4	$CuCl_2•2H_2O$	38

5	$CuBr_2$	29
6	$CuSO_4•5H_2O$	27
7	CuI	42
8	$Co(acac)_2$	N.D
9	$CoCl_2$	1
10	$CoCO_3$	45
11	$Co(OAc)_2$	N.D
12	$Co(NO_3)_2•6H_2O$	26
13	$Fe(acac)_3$	10
14	$Fe(OTs)_3•6H_2O$	17
15	Feox	22
16	$FeCl_3$	19
17	$FeSO_4•7H_2O$	24
18	$Ni(acac)_2$	N.D
19	$Ni(OTf)_2$	1
20	$NiCl_2$	N.D
21	$Ni(OAc)_2•4H_2O$	N.D
22	$NiCO_3$	N.D

Reaction conditions: [a] **1a** (0.2 mmol), **2a** (0.2 mmol), **3a** (0.6 mmol)， **4a** (0.6 mmol)， catalyst (10 mol%), DPPE (15 mol%), DCE (2 mL), T =120 °C, t=4 h. [b] Isolated yield. [c] N.D means not detected.

Table S3 Screening of ligand [a, b, c]

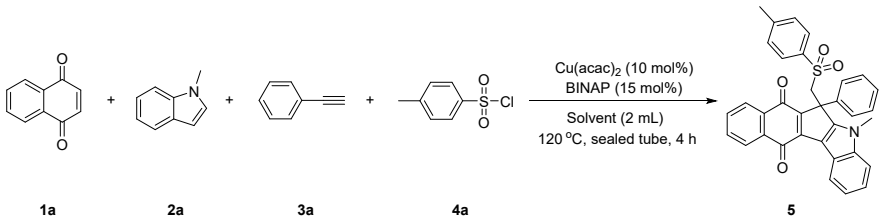


Entry	Ligand	Yield (%)
1	NEt_3	35

2	Py	12
3	CH_3COOH	29
4	CF_3COOH	42
5	PPh_3	17
6	Bipy	19
7	1,10-Phen	44
8	8-Hydroxyquinoline	36
9	BINAP	56
10	DPEPhos	30

Reaction conditions: [a] **1a** (0.2 mmol), **2a** (0.2 mmol), **3a** (0.6 mmol)，**4a** (0.6 mmol)，$Cu(acac)_2$ (10 mol%), ligand (15 mol%), DCE (2 mL), T =120 °C, t=4 h. [b] Isolated yield. [c] N.D means not detected. Bis[2-(diphenylphosphino)phenyl] Ether=DPEPhos, 1.1'-Binaphthyl-2.2'-diphemyl phosphine=BINAP.

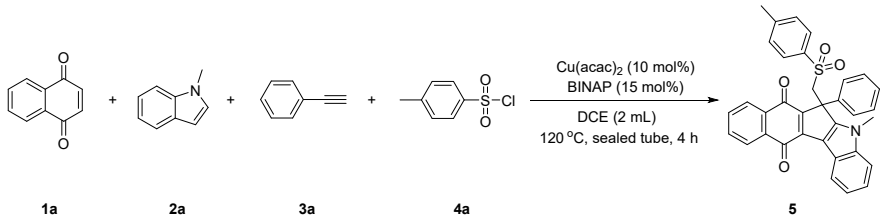
Table S4 Screening of solvent [a, b, c]



Entry	Solvent	Yield (%)
1	DCE	56
2	CH_3CN	48
3	EA	19
4	1,4-dioxane	7
5	toluene	12
6	DMSO	N.D
7	DMF	N.D
8	THF	8
9	$CHCl_3$	9

Reaction conditions: [a] **1a** (0.2 mmol), **2a** (0.2 mmol), **3a** (0.6 mmol)，**4a** (0.6 mmol)，$Cu(acac)_2$ (10 mol%), BINAP (15 mol%), solvent (2 mL), T =120 °C, t=4 h. [b] Isolated yield. [c] N.D means not detected.

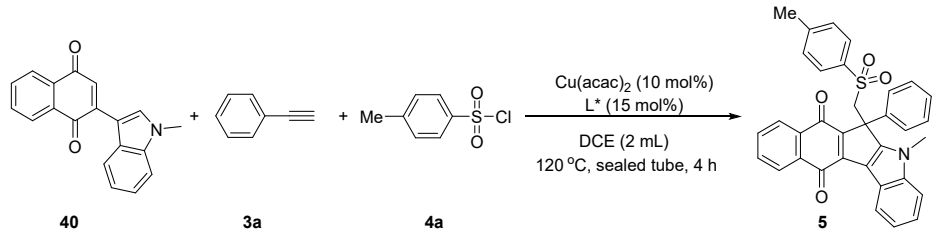
Table S5 Screening the ratio of substrate [a, b]

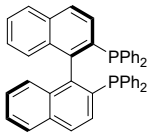
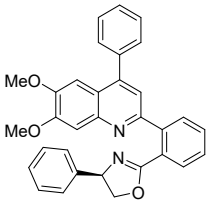
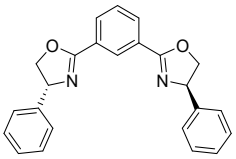
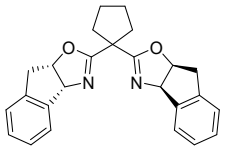
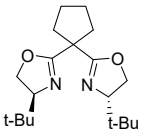
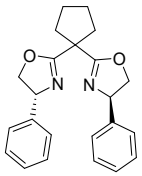
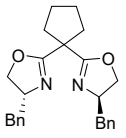
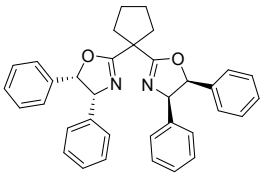
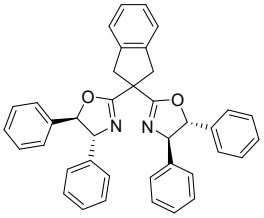
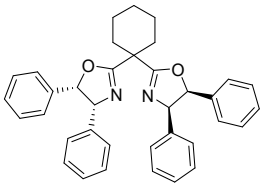
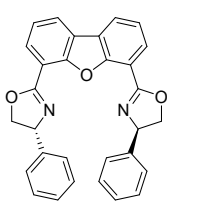
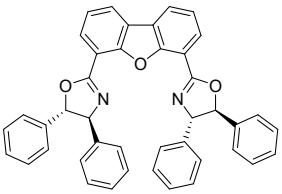
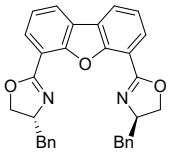
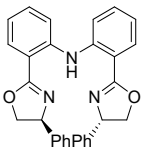
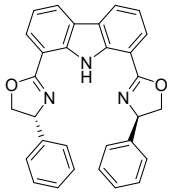


Entry	1a	2a	3a	4a	Yield (%)
1	0.4	0.2	0.6	0.6	32
2	0.2	0.4	0.6	0.6	40
3	0.4	0.4	0.2	0.6	29
4	0.4	0.4	0.6	0.2	21
5	0.2	0.2	0.2	0.2	20
6	**0.2**	**0.2**	**0.6**	**0.6**	**56**

Reaction conditions: [a] **1a** (x mmol), **2a** (y mmol), **3a** (z mmol)，**4a** (m mmol)，$Cu(acac)_2$ (10 mol%), BINAP (15 mol%), DCE (2 mL), T =120 °C, t=4 h. [b] Isolated yield.

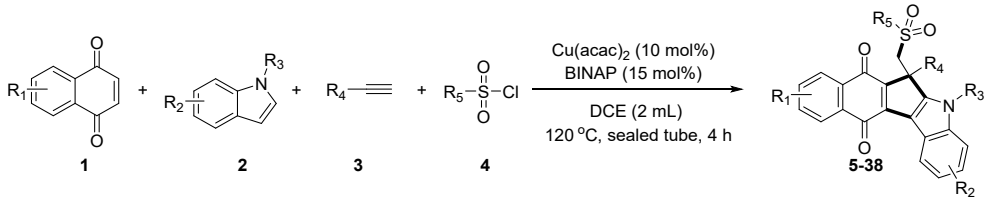
Table S6 Screening of chiral ligand [a, b]



			
L1 78% (2% ee)	L2 79% (0% ee)	L3 43% (2% ee)	L4 71% (11% ee)
			
L5 75% (-4% ee)	L6 45% (0% ee)	L7 75% (0% ee)	L8 77% (0% ee)
			
L9 68% (1% ee)	L10 80% (0% ee)	L11 56% (40% ee)	L12 34% (7% ee)
			
L13 56% (-40% ee)	L14 66% (6% ee)	L15 56% (15% ee)	

Reaction conditions: [a] **40** (0.2 mmol), **3a** (0.6 mmol)，**4a** (0.6 mmol)，$Cu(acac)_2$ (10 mol%), L* (15 mol%), DCE (2 mL), T =120 °C, t=4 h. [b] Isolated yield.

2.2 General procedures for the Synthesis of Products



Quinone (0.2 mmol, 1.0 equiv), indole (0.2 mmol, 1.0 equiv), alkyne (0.6 mmol, 3.0 equiv), sulfonyl chloride (0.6 mmol, 3.0 equiv), $Cu(acac)_2$ (10 mol%), BINAP (15 mol%) were sequentially added into the reaction flask and immediately dissolve them with 2 mL DCE, and the mixture was heated to 120 °C and stirred in the oil bath. After the reaction was completed, the solution was diluted with water and extracted three times with DCM. The organic phase was dried with anhydrous magnesium sulfate. The solvent was evaporated to dryness under reduced pressure, and the product was purified by column chromatography using ethyl acetate/petroleum ether as the eluent to obtain product. If the product is not pure, it can be recrystallized with ethyl acetate and petroleum ether.

3. X-Ray Crystallographic Data

3.1 X-Ray Crystallographic Data of 5

Single crystals of $C_{34}H_{25}NO_4S$ **5** were grown from ethyl acetate and PE. The ellipsoids are shown at 50% probability levels. A suitable crystal was selected and collected at 170.00 (10) K on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. The data were collected and processed using CrysAlisPro. The structures were solved by direct methods using Olex2 software with the SHELXT structure solution program via intrinsic phasing algorithm, and the non-hydrogen atoms were located from the trial structure and then refined anisotropically with SHELXL-2018 using a full-matrix least squares procedure based on F^2. The weighted R factor, wR and goodness-of-fit S values were obtained based on F^2. The hydrogen atom positions were fixed geometrically at the calculated distances and allowed to ride on their parent atoms. Crystallographic data for the structure reported in this paper have been deposited at the Cambridge Crystallographic Data Center and allocated with the deposition numbers: CCDC 2322361 for compound **5**.

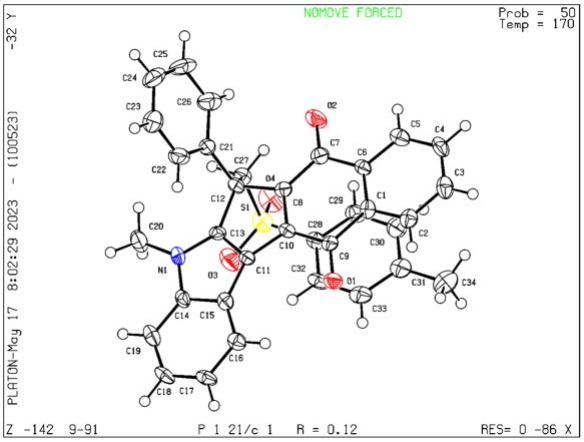


Figure S1 ORTEP Drawing of **5**

(The ellipsoids are shown at 50% probability levels)

Table S7 Crystal data and structure refinement for 5.

Identification code	5
Empirical formula	$C_{34}H_{25}NO_4S$
Formula weight	543.61

Temperature/K	170.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	18.415(2)
b/Å	10.7614(11)
c/Å	13.5967(18)
α/°	90
β/°	106.405(14)
γ/°	90
Volume/Å^3	2584.7(6)
Z	4
ρ_{calc}g/cm^3	1.397
μ/mm^{-1}	0.168
F(000)	1136.0
Crystal size/mm^3	0.15 × 0.14 × 0.11
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.432 to 49.996
Index ranges	-21 ≤ h ≤ 18, -10 ≤ k ≤ 12, -16 ≤ l ≤ 16
Reflections collected	10884
Independent reflections	4554 [R_{int} = 0.0550, R_{sigma} = 0.0730]
Data/restraints/parameters	4554/0/363
Goodness-of-fit on F^2	1.159
Final R indexes [I>=2σ (I)]	R_1 = 0.1191, wR_2 = 0.2476
Final R indexes [all data]	R_1 = 0.1427, wR_2 = 0.2592
Largest diff. peak/hole / e Å^{-3}	0.51/-0.59

Crystal structure determination of 5

Crystal Data for $C_{34}H_{25}NO_4S$ (M =543.61 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 18.415(2) Å, b = 10.7614(11) Å, c = 13.5967(18) Å, β = 106.405(14)°, V = 2584.7(6) Å^3, Z = 4, T = 170.00(10) K, μ(Mo Kα) = 0.168 mm^{-1}, $Dcalc$ = 1.397 g/cm^3, 10884 reflections measured (4.432° ≤ 2Θ ≤ 49.996°), 4554 unique (R_{int} = 0.0550, R_{sigma} = 0.0730) which were used in all calculations. The final R_1 was 0.1191 (I > 2σ(I)) and wR_2 was 0.2592 (all data).

Refinement model description

Table S8 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)

Table S8 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	3492.6(11)	3094.8(17)	4804.5(14)	34.4(5)
O1	775(2)	5893(4)	4905(3)	29.3(11)
O2	3571(3)	5231(5)	7480(4)	42.5(13)
O3	3276(3)	3277(5)	3706(4)	43.2(13)
O4	4049(3)	2168(5)	5265(4)	46.9(14)
N1	2991(3)	6035(5)	3218(4)	25.9(12)
C1	1518(3)	5532(5)	6619(5)	21.9(14)
C2	896(4)	5472(6)	7010(5)	28.9(15)
C3	995(4)	5219(7)	8043(5)	35.1(17)
C4	1715(4)	5008(6)	8682(5)	32.4(16)
C5	2337(4)	5058(6)	8301(5)	29.0(15)
C6	2253(4)	5338(6)	7277(5)	23.1(14)
C7	2929(4)	5403(6)	6896(5)	27.4(15)
C8	2796(3)	5658(6)	5813(5)	22.7(13)
C9	1405(3)	5763(5)	5511(5)	20.5(13)
C10	2092(3)	5827(5)	5158(4)	18.8(13)
C11	2142(3)	5965(5)	4133(4)	20.5(13)
C12	3407(3)	5727(6)	5242(5)	25.3(14)
C13	2889(3)	5891(6)	4162(5)	22.8(14)
C14	2274(4)	6138(6)	2540(5)	25.0(14)
C15	1717(4)	6124(6)	3079(5)	23.4(14)
C16	954(4)	6236(6)	2540(5)	27.4(15)
C17	760(4)	6335(6)	1483(5)	29.6(15)
C18	1312(4)	6339(6)	959(5)	28.7(15)
C19	2071(4)	6262(6)	1470(5)	32.3(16)
C20	3698(4)	5992(8)	2945(5)	39.1(18)
C21	3924(4)	6858(6)	5593(5)	24.4(14)
C22	3731(4)	7991(7)	5111(5)	38.9(18)
C23	4182(5)	9046(7)	5431(6)	47(2)
C24	4839(4)	8955(9)	6209(6)	48(2)
C25	5038(4)	7847(9)	6726(6)	47(2)
C26	4584(4)	6784(8)	6414(6)	41.2(19)
C27	3899(4)	4512(6)	5410(5)	29.1(15)
C28	2674(4)	2790(6)	5188(5)	28.1(15)
C29	2747(4)	2318(6)	6174(5)	34.3(17)
C30	2115(4)	2106(7)	6483(6)	37.8(18)
C31	1385(4)	2364(6)	5841(5)	31.8(16)

Table S8 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 5. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C32	1965(4)	3019(6)	4527(5)	30.7(16)
C33	1326(4)	2815(6)	4846(5)	32.1(16)
C34	702(4)	2154(7)	6193(7)	45(2)

Table S9 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 5. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	43.0(10)	29.0(9)	31.9(10)	0.2(8)	11.6(8)	5.3(8)
O1	24(2)	37(3)	24(2)	0(2)	2.4(19)	1(2)
O2	32(3)	66(4)	25(3)	11(3)	0(2)	4(3)
O3	59(3)	44(3)	30(3)	-2(2)	17(2)	0(3)
O4	57(3)	33(3)	52(3)	4(3)	17(3)	17(3)
N1	31(3)	26(3)	22(3)	7(2)	10(2)	-1(2)
C1	30(3)	8(3)	29(3)	7(2)	9(3)	3(3)
C2	32(4)	25(4)	33(4)	-3(3)	13(3)	-2(3)
C3	41(4)	36(4)	35(4)	0(3)	22(3)	0(3)
C4	53(5)	28(4)	20(3)	-3(3)	16(3)	-6(3)
C5	39(4)	20(3)	24(3)	1(3)	3(3)	3(3)
C6	33(4)	16(3)	18(3)	1(2)	3(3)	-2(3)
C7	28(3)	23(3)	28(4)	4(3)	2(3)	-1(3)
C8	23(3)	18(3)	25(3)	1(3)	3(3)	0(3)
C9	25(3)	11(3)	23(3)	-2(2)	4(3)	-2(3)
C10	28(3)	10(3)	16(3)	-1(2)	3(2)	1(2)
C11	28(3)	15(3)	17(3)	0(2)	3(3)	-2(3)
C12	24(3)	29(4)	19(3)	8(3)	1(3)	2(3)
C13	28(3)	18(3)	19(3)	0(3)	0(3)	-6(3)
C14	35(4)	19(3)	21(3)	5(3)	9(3)	-2(3)
C15	34(3)	13(3)	24(3)	1(3)	9(3)	0(3)
C16	32(4)	23(3)	25(3)	2(3)	5(3)	3(3)
C17	41(4)	21(3)	19(3)	2(3)	-3(3)	1(3)
C18	49(4)	20(3)	14(3)	2(3)	3(3)	4(3)
C19	50(4)	26(4)	24(4)	4(3)	16(3)	2(3)
C20	35(4)	55(5)	29(4)	13(4)	13(3)	6(4)
C21	31(3)	19(3)	23(3)	-2(3)	7(3)	-5(3)
C22	41(4)	38(4)	29(4)	6(3)	-4(3)	-8(3)
C23	61(5)	31(4)	46(5)	7(4)	9(4)	-19(4)

Table S9 Anisotropic Displacement Parameters ($Å^2×10^3$) for 5. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C24	37(4)	60(6)	50(5)	-26(4)	18(4)	-23(4)
C25	20(4)	66(6)	48(5)	-21(4)	0(3)	-3(4)
C26	30(4)	51(5)	38(4)	-8(4)	3(3)	2(4)
C27	29(3)	30(4)	26(4)	2(3)	5(3)	-1(3)
C28	36(4)	21(3)	25(4)	2(3)	3(3)	1(3)
C29	38(4)	29(4)	29(4)	8(3)	-1(3)	-2(3)
C30	47(4)	29(4)	36(4)	1(3)	10(3)	-7(3)
C31	42(4)	15(3)	36(4)	-3(3)	7(3)	-2(3)
C32	48(4)	17(3)	21(3)	-3(3)	-2(3)	0(3)
C33	41(4)	19(3)	32(4)	-6(3)	2(3)	-1(3)
C34	42(4)	31(4)	61(6)	-6(4)	14(4)	-1(4)

Table S10 Bond Lengths for 5.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O3	1.446(5)	C11	C15	1.435(8)
S1	O4	1.439(5)	C12	C13	1.519(8)
S1	C27	1.793(7)	C12	C21	1.536(9)
S1	C28	1.760(7)	C12	C27	1.570(9)
O1	C9	1.227(7)	C14	C15	1.420(9)
O2	C7	1.238(8)	C14	C19	1.403(9)
N1	C13	1.356(8)	C15	C16	1.395(9)
N1	C14	1.384(8)	C16	C17	1.384(9)
N1	C20	1.453(8)	C17	C18	1.395(10)
C1	C2	1.392(9)	C18	C19	1.377(10)
C1	C6	1.412(9)	C21	C22	1.382(9)
C1	C9	1.482(8)	C21	C26	1.402(9)
C2	C3	1.392(9)	C22	C23	1.402(10)
C3	C4	1.384(10)	C23	C24	1.367(11)
C4	C5	1.385(10)	C24	C25	1.380(12)
C5	C6	1.389(9)	C25	C26	1.410(11)
C6	C7	1.480(9)	C28	C29	1.405(9)
C7	C8	1.449(9)	C28	C32	1.382(9)
C8	C10	1.361(8)	C29	C30	1.364(10)
C8	C12	1.539(9)	C30	C31	1.408(10)
C9	C10	1.476(8)	C31	C33	1.412(10)
C10	C11	1.430(8)	C31	C34	1.484(10)

Table S10 Bond Lengths for 5.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C11	C13	1.368(9)	C32	C33	1.381(10)

Table S11 Bond Angles for 5.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O3	S1	C27	108.5(3)	C13	C12	C21	111.9(5)
O3	S1	C28	108.8(3)	C13	C12	C27	114.6(5)
O4	S1	O3	119.9(3)	C21	C12	C8	111.1(5)
O4	S1	C27	103.6(3)	C21	C12	C27	109.5(5)
O4	S1	C28	107.8(3)	N1	C13	C11	111.9(5)
C28	S1	C27	107.7(3)	N1	C13	C12	135.4(6)
C13	N1	C14	106.2(5)	C11	C13	C12	112.7(5)
C13	N1	C20	127.6(5)	N1	C14	C15	110.3(5)
C14	N1	C20	126.0(5)	N1	C14	C19	128.6(6)
C2	C1	C6	119.7(6)	C19	C14	C15	121.1(6)
C2	C1	C9	120.1(6)	C14	C15	C11	104.3(5)
C6	C1	C9	120.2(5)	C16	C15	C11	135.9(6)
C3	C2	C1	120.5(6)	C16	C15	C14	119.7(6)
C4	C3	C2	119.6(6)	C17	C16	C15	118.6(6)
C5	C4	C3	120.5(6)	C16	C17	C18	121.3(6)
C4	C5	C6	120.8(6)	C19	C18	C17	121.6(6)
C1	C6	C7	121.5(5)	C18	C19	C14	117.7(6)
C5	C6	C1	118.9(6)	C22	C21	C12	119.9(6)
C5	C6	C7	119.6(6)	C22	C21	C26	118.5(6)
O2	C7	C6	120.9(6)	C26	C21	C12	121.6(6)
O2	C7	C8	122.5(6)	C21	C22	C23	121.1(7)
C8	C7	C6	116.5(5)	C24	C23	C22	120.0(8)
C7	C8	C12	125.7(5)	C23	C24	C25	120.4(7)
C10	C8	C7	123.2(6)	C24	C25	C26	119.9(7)
C10	C8	C12	111.1(5)	C21	C26	C25	120.0(8)
O1	C9	C1	122.4(5)	C12	C27	S1	119.5(5)
O1	C9	C10	120.8(5)	C29	C28	S1	119.4(5)
C10	C9	C1	116.9(5)	C32	C28	S1	120.3(5)
C8	C10	C9	121.7(5)	C32	C28	C29	120.3(7)
C8	C10	C11	109.9(5)	C30	C29	C28	119.5(6)
C11	C10	C9	128.2(5)	C29	C30	C31	121.7(7)
C10	C11	C15	144.9(6)	C30	C31	C33	117.6(7)
C13	C11	C10	107.9(5)	C30	C31	C34	121.1(7)

Table S11 Bond Angles for 5.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C13	C11	C15	107.2(5)	C33	C31	C34	121.2(7)
C8	C12	C27	111.1(5)	C33	C32	C28	119.9(6)
C13	C12	C8	98.3(5)	C32	C33	C31	120.9(6)

Table S12 Torsion Angles for 5.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	C28	C29	C30	178.6(6)	C10	C11	C13	N1	-178.9(5)
S1	C28	C32	C33	-177.9(5)	C10	C11	C13	C12	-1.5(7)
O1	C9	C10	C8	-178.5(6)	C10	C11	C15	C14	-178.2(8)
O1	C9	C10	C11	-3.7(9)	C10	C11	C15	C16	0.8(15)
O2	C7	C8	C10	178.8(6)	C11	C15	C16	C17	-177.6(7)
O2	C7	C8	C12	1.2(10)	C12	C8	C10	C9	178.0(5)
O3	S1	C27	C12	61.1(6)	C12	C8	C10	C11	2.4(7)
O3	S1	C28	C29	166.3(5)	C12	C21	C22	C23	178.5(7)
O3	S1	C28	C32	-14.1(6)	C12	C21	C26	C25	-178.9(6)
O4	S1	C27	C12	-170.5(5)	C13	N1	C14	C15	3.1(7)
O4	S1	C28	C29	34.8(6)	C13	N1	C14	C19	-177.8(7)
O4	S1	C28	C32	-145.5(5)	C13	C11	C15	C14	-0.3(7)
N1	C14	C15	C11	-1.8(7)	C13	C11	C15	C16	178.7(7)
N1	C14	C15	C16	179.1(6)	C13	C12	C21	C22	20.5(9)
N1	C14	C19	C18	179.5(6)	C13	C12	C21	C26	-161.2(6)
C1	C2	C3	C4	-1.0(10)	C13	C12	C27	S1	-38.7(7)
C1	C6	C7	O2	-180.0(6)	C14	N1	C13	C11	-3.4(7)
C1	C6	C7	C8	-0.8(9)	C14	N1	C13	C12	-180.0(7)
C1	C9	C10	C8	1.2(8)	C14	C15	C16	C17	1.2(9)
C1	C9	C10	C11	176.0(6)	C15	C11	C13	N1	2.3(7)
C2	C1	C6	C5	1.7(9)	C15	C11	C13	C12	179.7(5)
C2	C1	C6	C7	-179.5(6)	C15	C14	C19	C18	-1.5(10)
C2	C1	C9	O1	-0.9(9)	C15	C16	C17	C18	-0.8(10)
C2	C1	C9	C10	179.4(5)	C16	C17	C18	C19	-0.9(10)
C2	C3	C4	C5	0.6(11)	C17	C18	C19	C14	2.0(10)
C3	C4	C5	C6	0.9(10)	C19	C14	C15	C11	179.1(6)
C4	C5	C6	C1	-2.0(9)	C19	C14	C15	C16	-0.1(9)
C4	C5	C6	C7	179.2(6)	C20	N1	C13	C11	-178.9(6)
C5	C6	C7	O2	-1.2(10)	C20	N1	C13	C12	4.6(12)
C5	C6	C7	C8	178.0(6)	C20	N1	C14	C15	178.7(6)
C6	C1	C2	C3	-0.2(9)	C20	N1	C14	C19	-2.2(11)

Table S12 Torsion Angles for 5.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C6	C1	C9	O1	177.4(6)	C21	C12	C13	N1	62.5(10)
C6	C1	C9	C10	-2.4(8)	C21	C12	C13	C11	-114.1(6)
C6	C7	C8	C10	-0.4(9)	C21	C12	C27	S1	-165.4(5)
C6	C7	C8	C12	-178.0(6)	C21	C22	C23	C24	2.2(13)
C7	C8	C10	C9	0.1(9)	C22	C21	C26	C25	-0.6(11)
C7	C8	C10	C11	-175.5(6)	C22	C23	C24	C25	-4.0(13)
C7	C8	C12	C13	174.9(6)	C23	C24	C25	C26	3.6(12)
C7	C8	C12	C21	-67.7(8)	C24	C25	C26	C21	-1.2(11)
C7	C8	C12	C27	54.4(8)	C26	C21	C22	C23	0.2(11)
C8	C10	C11	C13	-0.6(7)	C27	S1	C28	C29	-76.4(6)
C8	C10	C11	C15	177.4(8)	C27	S1	C28	C32	103.3(6)
C8	C12	C13	N1	179.2(7)	C27	C12	C13	N1	-62.9(9)
C8	C12	C13	C11	2.7(7)	C27	C12	C13	C11	120.5(6)
C8	C12	C21	C22	-88.2(7)	C27	C12	C21	C22	148.7(6)
C8	C12	C21	C26	90.0(7)	C27	C12	C21	C26	-33.0(8)
C8	C12	C27	S1	71.6(6)	C28	S1	C27	C12	-56.4(6)
C9	C1	C2	C3	178.1(6)	C28	C29	C30	C31	-0.8(11)
C9	C1	C6	C5	-176.6(6)	C28	C32	C33	C31	-0.5(10)
C9	C1	C6	C7	2.2(9)	C29	C28	C32	C33	1.7(10)
C9	C10	C11	C13	-175.9(6)	C29	C30	C31	C33	2.0(10)
C9	C10	C11	C15	2.1(13)	C29	C30	C31	C34	-178.7(7)
C10	C8	C12	C13	-3.0(7)	C30	C31	C33	C32	-1.4(10)
C10	C8	C12	C21	114.4(6)	C32	C28	C29	C30	-1.1(10)
C10	C8	C12	C27	-123.5(6)	C34	C31	C33	C32	179.4(6)

Table S13 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5.

Atom	*x*	*y*	*z*	U(eq)
H2	401.6	5605.21	6567.62	35
H3	569.8	5191.55	8308.69	42
H4	1783.88	4826.53	9385.91	39
H5	2827.99	4899.55	8745.28	35
H16	575.15	6243.78	2891.45	33
H17	241.89	6401.5	1106.91	35
H18	1159.41	6396.05	232.29	34
H19	2444.14	6291.78	1109.85	39
H20A	4117.72	6211.34	3544.37	59

Table S13 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5.

Atom	*x*	*y*	*z*	U(eq)
H20B	3677.75	6584.53	2390.51	59
H20C	3776.66	5151.95	2716.81	59
H22	3284.23	8056.72	4554.57	47
H23	4032.33	9824.01	5107.46	57
H24	5160.53	9658.08	6395.5	57
H25	5480.14	7800.8	7291.5	56
H26	4725.95	6016.26	6760.61	49
H27A	4074.83	4355.06	6157.63	35
H27B	4354.13	4687.77	5183.46	35
H29	3234.67	2147.33	6623.94	41
H30	2167.99	1776.64	7147.5	45
H32	1916.83	3316.84	3853.73	37
H33	840.49	2979.63	4389.89	39
H34A	500.28	1321.94	5985.24	67
H34B	318.04	2778.15	5885.47	67
H34C	838.17	2222.48	6941.9	67

3.2 X-Ray Crystallographic Data of 41

Single crystals of $C_{38}H_{33}NO_6S$ **41** were grown from ethyl acetate and PE. The ellipsoids are shown at 50% probability levels. A suitable crystal was selected and collected at 170.00 (10) K on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. The data were collected and processed using CrysAlisPro. The structures were solved by direct methods using Olex2 software with the SHELXT structure solution program via intrinsic phasing algorithm, and the non-hydrogen atoms were located from the trial structure and then refined anisotropically with SHELXL-2018 using a full-matrix least squares procedure based on F^2. The weighted *R* factor, *wR* and goodness-of-fit *S* values were obtained based on F^2. The hydrogen atom positions were fixed geometrically at the calculated distances and allowed to ride on their parent atoms. Crystallographic data for the structure reported in this paper have been deposited at the Cambridge Crystallographic Data Center and allocated with the deposition numbers: CCDC 2322362 for compound **41**.

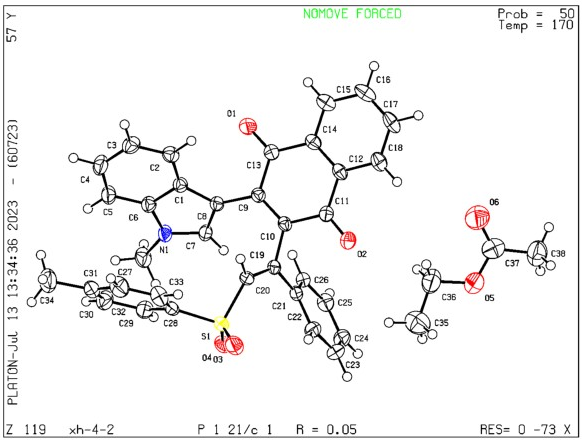


Figure S1 ORTEP Drawing of **41**

(The ellipsoids are shown at 50% probability levels)

Table S14 Crystal data and structure refinement for 41.

Identification code	41
Empirical formula	$C_{38}H_{33}NO_6S$
Formula weight	631.71
Temperature/K	170.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$

a/Å	8.4208(6)
b/Å	32.501(2)
c/Å	11.8454(8)
α/°	90
β/°	104.606(7)
γ/°	90
Volume/Å^3	3137.2(4)
Z	4
ρ_{calc}g/cm^3	1.337
μ/mm^{-1}	0.154
F(000)	1328.0
Crystal size/mm^3	0.15 × 0.14 × 0.12
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.348 to 49.996
Index ranges	-9 ≤ h ≤ 10, -38 ≤ k ≤ 35, -13 ≤ l ≤ 14
Reflections collected	14125
Independent reflections	5500 [R_{int} = 0.0315, R_{sigma} = 0.0463]
Data/restraints/parameters	5500/0/419
Goodness-of-fit on F^2	1.017
Final R indexes [I>=2σ (I)]	R_1 = 0.0511, wR_2 = 0.1157
Final R indexes [all data]	R_1 = 0.0672, wR_2 = 0.1253
Largest diff. peak/hole / e Å^{-3}	0.41/-0.40

Crystal structure determination of 41

Crystal Data for $C_{38}H_{33}NO_6S$ (*M* =631.71 g/mol): monoclinic, space group $P2_1/c$ (no. 14), *a* = 8.4208(6) Å, *b* = 32.501(2) Å, *c* = 11.8454(8) Å, *β* = 104.606(7)°, *V* = 3137.2(4) Å^3, *Z* = 4, *T* = 170.00(10) K, μ(Mo Kα) = 0.154 mm^{-1}, *Dcalc* = 1.337 g/cm^3, 14125 reflections measured (4.348° ≤ 2Θ ≤ 49.996°), 5500 unique (R_{int} = 0.0315, R_{sigma} = 0.0463) which were used in all calculations. The final R_1 was 0.0511 (I > 2σ(I)) and wR_2 was 0.1253 (all data).

Refinement model description

Table S15 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 41. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	7244.5(7)	3336.9(2)	5419.5(5)	27.35(16)
O1	2472(2)	4335.7(6)	8513.1(16)	50.0(5)
O2	3746(2)	4618.2(5)	4406.3(15)	39.9(5)
O3	8487(2)	3489.9(6)	4894.1(16)	44.2(5)

Table S15 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 41. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O4	6150(2)	3027.2(5)	4806.7(14)	38.4(4)
N1	4134(2)	3005.9(6)	7959.8(16)	31.1(5)
C1	4817(3)	3622.0(7)	8822.4(19)	25.3(5)
C2	5581(3)	3878.6(8)	9753(2)	30.5(5)
C3	6395(3)	3703.3(8)	10793(2)	35.2(6)
C4	6480(3)	3276.1(8)	10936(2)	39.4(6)
C5	5754(3)	3015.8(8)	10046(2)	35.3(6)
C6	4926(3)	3194.0(7)	8993.1(19)	28.1(5)
C7	3564(3)	3303.1(7)	7156(2)	28.9(5)
C8	3936(3)	3687.5(7)	7622.1(19)	24.8(5)
C9	3534(3)	4079.7(7)	6993.9(18)	23.9(5)
C10	3805(3)	4155.8(7)	5929.2(18)	22.9(5)
C11	3372(3)	4555.3(7)	5323.0(19)	26.6(5)
C12	2534(3)	4870.1(7)	5864(2)	26.9(5)
C13	2726(3)	4402.2(8)	7562(2)	29.1(5)
C14	2218(3)	4794.7(7)	6947(2)	27.9(5)
C15	1412(3)	5087.5(8)	7448(2)	37.4(6)
C16	926(3)	5452.9(8)	6870(3)	43.1(7)
C17	1255(3)	5531.4(8)	5803(3)	43.2(7)
C18	2060(3)	5241.1(8)	5300(2)	36.1(6)
C19	4579(3)	3847.8(7)	5300.6(18)	23.2(5)
C20	6135(3)	3750.1(7)	5782.9(19)	24.2(5)
C21	3503(3)	3692.4(7)	4186.4(19)	24.1(5)
C22	4055(3)	3660.2(8)	3180(2)	31.9(6)
C23	2988(3)	3542.9(8)	2137(2)	38.1(6)
C24	1371(3)	3454.1(8)	2091(2)	37.2(6)
C25	811(3)	3481.8(8)	3083(2)	32.7(6)
C26	1864(3)	3605.3(7)	4124.5(19)	27.2(5)
C27	3814(4)	2568.5(8)	7803(2)	42.4(7)
C28	8236(3)	3138.2(7)	6805.9(19)	26.8(5)
C29	7641(3)	2783.3(8)	7184(2)	34.8(6)
C30	8478(4)	2606.9(8)	8233(2)	42.6(7)
C31	9894(3)	2786.4(9)	8903(2)	41.8(7)
C32	10433(3)	3150.1(9)	8524(2)	44.4(7)
C33	9620(3)	3328.6(8)	7480(2)	37.1(6)
C34	10822(5)	2583.3(10)	10019(3)	66.5(10)

Table S15 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 41. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O5	2083(3)	5226.5(7)	954.7(17)	55.5(5)
O6	1577(3)	5671.2(7)	2232.0(19)	69.1(7)
C35	4105(4)	4707.9(11)	1420(3)	65.8(9)
C36	3108(4)	4997.0(11)	1920(3)	59.9(9)
C37	1392(4)	5560.2(10)	1248(3)	48.0(7)
C38	351(4)	5774.2(11)	200(3)	61.9(9)

Table S16 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 41. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	31.5(3)	22.4(3)	29.0(3)	0.1(3)	9.2(2)	4.6(2)
O1	66.9(13)	50.9(13)	41.0(11)	12.2(10)	30.2(10)	26.0(10)
O2	58.5(12)	31.1(10)	33.7(10)	8.8(8)	18.2(9)	7.3(8)
O3	46.3(11)	42.7(11)	52.9(11)	14.2(9)	29.6(9)	12.4(9)
O4	50.9(11)	24.2(9)	33.4(9)	-6.7(8)	-1.8(8)	5.9(8)
N1	43.0(12)	20.4(11)	25.8(10)	1.7(9)	1.2(9)	0.5(9)
C1	25.3(12)	25.0(13)	26.1(12)	1.9(10)	7.1(10)	0.4(10)
C2	32.7(13)	25.4(13)	34.3(13)	-0.9(11)	10.2(11)	-2.3(11)
C3	39.6(15)	35.9(15)	27.6(13)	-4.8(11)	3.9(11)	-6.1(12)
C4	44.6(16)	40.1(16)	27.8(13)	6.4(12)	-1.5(11)	1.2(13)
C5	44.2(15)	27.2(14)	30.5(13)	5.2(11)	2.1(11)	2.0(11)
C6	31.1(13)	25.3(13)	26.9(12)	1.5(10)	5.3(10)	-0.6(10)
C7	36.7(14)	25.4(13)	22.4(11)	2.9(10)	3.2(10)	1.6(10)
C8	27.5(12)	23.0(13)	25.2(12)	2.9(10)	9.1(10)	2.0(10)
C9	25.2(12)	21.4(12)	24.4(12)	-0.2(10)	4.6(9)	0.5(9)
C10	23.9(12)	17.9(12)	25.0(11)	-0.8(9)	2.6(9)	-0.7(9)
C11	28.4(12)	25.0(13)	24.9(12)	1.6(10)	4.0(10)	-1.2(10)
C12	24.5(12)	19.3(12)	34.9(13)	-0.8(10)	3.7(10)	-0.1(10)
C13	30.7(13)	28.5(14)	28.7(13)	2.3(11)	8.5(10)	3.7(10)
C14	26.3(12)	23.2(13)	33.3(13)	-3.1(11)	5.8(10)	0.7(10)
C15	37.7(14)	29.4(15)	46.3(15)	-4.4(12)	12.9(12)	3.4(12)
C16	42.8(16)	25.5(14)	62.9(18)	-8.7(14)	17.0(14)	5.5(12)
C17	44.3(16)	20.6(14)	64.5(19)	7.8(13)	13.3(14)	6.6(12)
C18	38.0(14)	25.4(14)	44.8(15)	5.9(12)	10.4(12)	2.1(11)
C19	27.1(12)	19.5(12)	24.0(11)	3.5(10)	8.5(10)	0.7(9)

Table S16 Anisotropic Displacement Parameters ($Å^2×10^3$) for 41. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C20	30.8(13)	16.7(12)	24.7(12)	-2.4(9)	6.1(10)	-0.7(9)
C21	26.2(12)	20.7(12)	23.9(12)	2.1(10)	3.7(9)	3.4(9)
C22	31.6(13)	36.4(15)	28.1(13)	1.0(11)	8.6(10)	2.6(11)
C23	48.6(16)	42.0(16)	24.3(13)	-2.2(12)	10.5(12)	4.6(13)
C24	42.3(16)	35.7(15)	27.8(13)	-4.1(11)	-2.0(11)	1.3(12)
C25	29.6(13)	30.3(14)	35.1(14)	-0.5(11)	2.7(11)	-2.0(11)
C26	30.2(13)	26.6(13)	24.7(12)	1.7(10)	6.7(10)	5.1(10)
C27	59.8(18)	21.3(14)	38.8(15)	-0.3(12)	-0.9(13)	-2.0(12)
C28	27.6(12)	22.9(13)	30.6(12)	-0.8(10)	8.8(10)	4.9(10)
C29	41.8(15)	28.0(14)	31.9(13)	-3.3(11)	4.4(11)	-4.6(11)
C30	62.5(18)	29.6(15)	33.3(14)	1.7(12)	7.5(13)	-2.1(13)
C31	52.0(17)	35.2(16)	33.1(14)	-1.9(12)	1.4(13)	15.0(13)
C32	32.0(14)	45.1(18)	47.6(16)	-5.8(14)	-5.8(12)	1.7(13)
C33	29.1(14)	30.3(15)	49.6(16)	2.4(12)	5.5(12)	-2.0(11)
C34	89(3)	52(2)	43.5(17)	1.8(16)	-12.1(17)	19.2(18)
O5	68.7(14)	55.3(14)	41.1(11)	3.4(10)	11.3(10)	4.9(11)
O6	83.2(17)	59.7(16)	54.4(14)	-14.0(12)	-1.2(12)	-6.5(13)
C35	57(2)	63(2)	74(2)	-13.2(19)	8.5(18)	0.6(17)
C36	67(2)	63(2)	45.3(18)	10.8(16)	5.4(16)	3.2(17)
C37	52.5(18)	44.0(18)	49.6(18)	-7.4(15)	16.6(14)	-16.8(15)
C38	54(2)	74(2)	59(2)	20.7(18)	16.9(16)	6.0(17)

Table S17 Bond Lengths for 41.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O3	1.4346(18)	C13	C14	1.478(3)
S1	O4	1.4327(18)	C14	C15	1.386(3)
S1	C20	1.750(2)	C15	C16	1.380(4)
S1	C28	1.766(2)	C16	C17	1.384(4)
O1	C13	1.218(3)	C17	C18	1.382(4)
O2	C11	1.222(3)	C19	C20	1.330(3)
N1	C6	1.380(3)	C19	C21	1.488(3)
N1	C7	1.356(3)	C21	C22	1.389(3)
N1	C27	1.450(3)	C21	C26	1.392(3)
C1	C2	1.402(3)	C22	C23	1.385(3)
C1	C6	1.405(3)	C23	C24	1.380(4)
C1	C8	1.444(3)	C24	C25	1.375(3)

Table S17 Bond Lengths for 41.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C2	C3	1.374(3)	C25	C26	1.385(3)
C3	C4	1.399(4)	C28	C29	1.377(3)
C4	C5	1.370(4)	C28	C33	1.382(3)
C5	C6	1.392(3)	C29	C30	1.388(3)
C7	C8	1.370(3)	C30	C31	1.384(4)
C8	C9	1.472(3)	C31	C32	1.381(4)
C9	C10	1.360(3)	C31	C34	1.508(4)
C9	C13	1.499(3)	C32	C33	1.381(4)
C10	C11	1.484(3)	O5	C36	1.453(3)
C10	C19	1.492(3)	O5	C37	1.318(4)
C11	C12	1.477(3)	O6	C37	1.192(3)
C12	C14	1.396(3)	C35	C36	1.480(5)
C12	C18	1.388(3)	C37	C38	1.498(4)

Table S18 Bond Angles for 41.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O3	S1	C20	109.50(11)	O1	C13	C14	120.8(2)
O3	S1	C28	107.72(11)	C14	C13	C9	119.4(2)
O4	S1	O3	118.05(12)	C12	C14	C13	120.4(2)
O4	S1	C20	110.39(11)	C15	C14	C12	120.0(2)
O4	S1	C28	107.89(11)	C15	C14	C13	119.6(2)
C20	S1	C28	102.03(10)	C16	C15	C14	119.7(3)
C6	N1	C27	125.50(19)	C15	C16	C17	120.6(2)
C7	N1	C6	108.25(19)	C18	C17	C16	120.1(2)
C7	N1	C27	125.9(2)	C17	C18	C12	119.9(2)
C2	C1	C6	118.4(2)	C20	C19	C10	116.9(2)
C2	C1	C8	134.9(2)	C20	C19	C21	127.9(2)
C6	C1	C8	106.6(2)	C21	C19	C10	115.19(18)
C3	C2	C1	119.0(2)	C19	C20	S1	127.38(18)
C2	C3	C4	121.3(2)	C22	C21	C19	121.7(2)
C5	C4	C3	121.4(2)	C22	C21	C26	118.8(2)
C4	C5	C6	117.3(2)	C26	C21	C19	119.31(19)
N1	C6	C1	108.16(19)	C23	C22	C21	120.2(2)
N1	C6	C5	129.1(2)	C24	C23	C22	120.3(2)
C5	C6	C1	122.7(2)	C25	C24	C23	120.0(2)
N1	C7	C8	111.2(2)	C24	C25	C26	120.0(2)
C1	C8	C9	128.4(2)	C25	C26	C21	120.6(2)

Table S18 Bond Angles for 41.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C7	C8	C1	105.7(2)	C29	C28	S1	118.91(18)
C7	C8	C9	125.9(2)	C29	C28	C33	120.7(2)
C8	C9	C13	116.82(19)	C33	C28	S1	120.39(19)
C10	C9	C8	123.8(2)	C28	C29	C30	119.6(2)
C10	C9	C13	119.4(2)	C31	C30	C29	120.6(3)
C9	C10	C11	122.0(2)	C30	C31	C34	120.0(3)
C9	C10	C19	122.5(2)	C32	C31	C30	118.8(2)
C11	C10	C19	115.50(18)	C32	C31	C34	121.3(3)
O2	C11	C10	119.3(2)	C31	C32	C33	121.4(2)
O2	C11	C12	121.9(2)	C32	C33	C28	119.0(2)
C12	C11	C10	118.81(19)	C37	O5	C36	115.4(2)
C14	C12	C11	120.0(2)	O5	C36	C35	107.2(3)
C18	C12	C11	120.2(2)	O5	C37	C38	111.6(3)
C18	C12	C14	119.8(2)	O6	C37	O5	123.3(3)
O1	C13	C9	119.8(2)	O6	C37	C38	125.1(3)

Table S19 Torsion Angles for 41.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	C28	C29	C30	175.28(19)	C10	C11	C12	C18	-177.7(2)
S1	C28	C33	C32	-175.59(19)	C10	C19	C20	S1	166.82(17)
O1	C13	C14	C12	179.1(2)	C10	C19	C21	C22	134.4(2)
O1	C13	C14	C15	-1.4(4)	C10	C19	C21	C26	-40.8(3)
O2	C11	C12	C14	-176.1(2)	C11	C10	C19	C20	113.2(2)
O2	C11	C12	C18	3.9(3)	C11	C10	C19	C21	-65.7(3)
O3	S1	C20	C19	111.6(2)	C11	C12	C14	C13	0.4(3)
O3	S1	C28	C29	-141.17(19)	C11	C12	C14	C15	-179.1(2)
O3	S1	C28	C33	36.6(2)	C11	C12	C18	C17	179.0(2)
O4	S1	C20	C19	-20.0(2)	C12	C14	C15	C16	0.0(4)
O4	S1	C28	C29	-12.7(2)	C13	C9	C10	C11	2.0(3)
O4	S1	C28	C33	165.09(19)	C13	C9	C10	C19	-179.0(2)
N1	C7	C8	C1	0.1(3)	C13	C14	C15	C16	-179.5(2)
N1	C7	C8	C9	178.7(2)	C14	C12	C18	C17	-1.0(4)
C1	C2	C3	C4	0.3(4)	C14	C15	C16	C17	-0.8(4)
C1	C8	C9	C10	131.3(2)	C15	C16	C17	C18	0.7(4)
C1	C8	C9	C13	-51.0(3)	C16	C17	C18	C12	0.2(4)
C2	C1	C6	N1	-178.3(2)	C18	C12	C14	C13	-179.6(2)
C2	C1	C6	C5	0.2(3)	C18	C12	C14	C15	0.9(3)

Table S19 Torsion Angles for 41.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C2	C1	C8	C7	177.3(2)	C19	C10	C11	O2	-4.2(3)
C2	C1	C8	C9	-1.3(4)	C19	C10	C11	C12	177.33(19)
C2	C3	C4	C5	-0.1(4)	C19	C21	C22	C23	-175.3(2)
C3	C4	C5	C6	-0.1(4)	C19	C21	C26	C25	176.4(2)
C4	C5	C6	N1	178.2(2)	C20	S1	C28	C29	103.6(2)
C4	C5	C6	C1	0.0(4)	C20	S1	C28	C33	-78.6(2)
C6	N1	C7	C8	-0.6(3)	C20	C19	C21	C22	-44.4(3)
C6	C1	C2	C3	-0.4(3)	C20	C19	C21	C26	140.4(2)
C6	C1	C8	C7	0.5(3)	C21	C19	C20	S1	-14.4(4)
C6	C1	C8	C9	-178.1(2)	C21	C22	C23	C24	-0.5(4)
C7	N1	C6	C1	0.9(3)	C22	C21	C26	C25	1.1(3)
C7	N1	C6	C5	-177.5(2)	C22	C23	C24	C25	0.0(4)
C7	C8	C9	C10	-47.0(3)	C23	C24	C25	C26	1.0(4)
C7	C8	C9	C13	130.6(2)	C24	C25	C26	C21	-1.6(4)
C8	C1	C2	C3	-176.9(2)	C26	C21	C22	C23	-0.1(4)
C8	C1	C6	N1	-0.8(3)	C27	N1	C6	C1	-173.0(2)
C8	C1	C6	C5	177.7(2)	C27	N1	C6	C5	8.7(4)
C8	C9	C10	C11	179.6(2)	C27	N1	C7	C8	173.2(2)
C8	C9	C10	C19	-1.4(3)	C28	S1	C20	C19	-134.4(2)
C8	C9	C13	O1	1.9(3)	C28	C29	C30	C31	0.5(4)
C8	C9	C13	C14	-177.0(2)	C29	C28	C33	C32	2.2(4)
C9	C10	C11	O2	174.9(2)	C29	C30	C31	C32	1.8(4)
C9	C10	C11	C12	-3.6(3)	C29	C30	C31	C34	-177.9(3)
C9	C10	C19	C20	-65.8(3)	C30	C31	C32	C33	-2.1(4)
C9	C10	C19	C21	115.2(2)	C31	C32	C33	C28	0.2(4)
C9	C13	C14	C12	-2.0(3)	C33	C28	C29	C30	-2.5(4)
C9	C13	C14	C15	177.5(2)	C34	C31	C32	C33	177.5(3)
C10	C9	C13	O1	179.7(2)	C36	O5	C37	O6	-0.1(4)
C10	C9	C13	C14	0.8(3)	C36	O5	C37	C38	-179.6(3)
C10	C11	C12	C14	2.3(3)	C37	O5	C36	C35	-165.1(3)

Table S20 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 41.

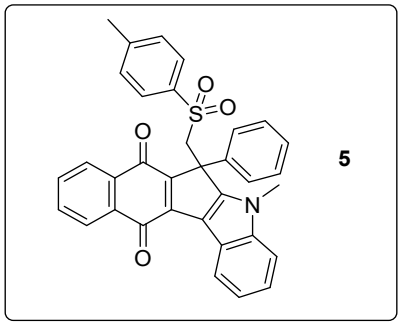
Atom	*x*	*y*	*z*	U(eq)
H2	5536.74	4169.24	9664.9	37
H3	6910.37	3875.63	11427.85	42
H4	7053.07	3163.99	11665.96	47

Table S20 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 41.

Atom	*x*	*y*	*z*	U(eq)
H5	5812.74	2725.54	10142.42	42
H7	2982.15	3251.37	6371.49	35
H15	1195.03	5036.99	8184.4	45
H16	361.32	5652.27	7208.35	52
H17	925.91	5785.12	5416.47	52
H18	2289.46	5295.43	4568.57	43
H20	6710.41	3924.25	6394.15	29
H22	5169.27	3718.79	3206.4	38
H23	3371.7	3523.41	1450.52	46
H24	644.07	3373.77	1373.56	45
H25	-298.45	3416.34	3054.04	39
H26	1465.18	3630.7	4803.28	33
H27A	4656.91	2414.72	8366.72	64
H27B	3837.87	2489.03	7009.02	64
H27C	2732.02	2506.01	7926.29	64
H29	6664.68	2660.1	6730.97	42
H30	8074.54	2360.82	8492.81	51
H32	11383.29	3280.23	8992	53
H33	10006.18	3578.57	7229.61	45
H34A	10206.34	2615.23	10614.4	100
H34B	11902.06	2712.63	10291.43	100
H34C	10959.81	2289.92	9877.76	100
H35A	3378.41	4517.93	886.13	99
H35B	4832.63	4551.45	2050.15	99
H35C	4764.85	4862.79	992.37	99
H36A	2418.35	4843.87	2340.86	72
H36B	3829.5	5186.68	2475.29	72
H38A	1057.98	5921.84	-206.13	93
H38B	-378.65	5970.06	447.94	93
H38C	-306.53	5570.57	-327.38	93

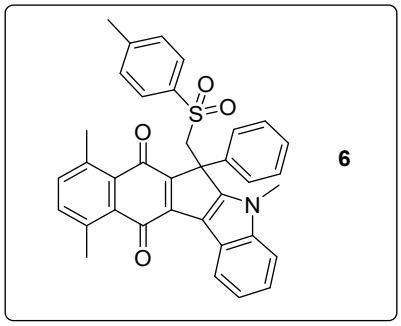
4. Characterization of compounds

5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (5)



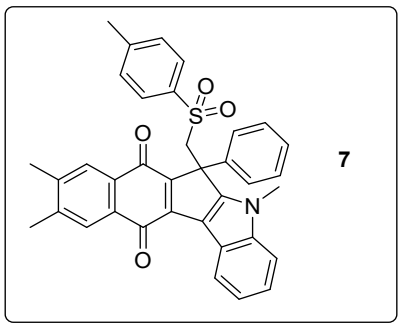
Blue solid, m.p. 243-244 °C, yield: 60.8 mg, 56% yield; Rf: 0.37 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.5 (dd, *J* = 5.5, 2.7 Hz, 1H), 8.0 (d, *J* = 8.9 Hz, 1H), 7.9 (d, *J* = 9.0 Hz, 1H), 7.7 – 7.6 (m, 2H), 7.4 (s, 3H), 7.2 (d, *J* = 6.5 Hz, 5H), 7.1 (dd, *J* = 6.4, 3.2 Hz, 2H), 6.7 (d, *J* = 7.9 Hz, 2H), 5.5 (d, *J* = 14.5 Hz, 1H), 4.4 (d, *J* = 14.5 Hz, 1H), 3.6 (s, 3H), 1.9 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.6, 178.7, 157.0, 146.5, 145.3, 143.0, 142.2, 136.2, 134.4, 134.1, 133.7, 132.2, 132.1, 129.3, 129.1, 128.5, 128.3, 125.8, 125.7, 125.6, 123.7, 122.7, 122.4, 121.7, 118.3, 110.6, 58.2, 52.5, 31.9, 21.2. HRMS (ESI) Calcd for $C_{34}H_{25}NNaO_4S^+$[M+Na]$^+$: 566.1402, Found: 566.1401.

5,8,11-trimethyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (6)



Purple solid, m.p. 260-261 °C, yield: 68.5 mg, 60% yield; Rf: 0.51 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.5 – 8.4 (m, 1H), 7.4 – 7.3 (m, 3H), 7.3 – 7.2 (m, 7H), 7.1 – 7.0 (m, 2H), 6.7 (d, *J* = 8.0 Hz, 2H), 5.5 (d, *J* = 14.6 Hz, 1H), 4.4 (d, *J* = 14.5 Hz, 1H), 3.6 (s, 3H), 2.8 (s, 3H), 2.6 (s, 3H), 1.9 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 185.0, 181.7, 156.3, 146.4, 145.1, 142.8, 142.3, 139.6, 139.3, 137.6, 136.6, 136.0, 134.7, 134.7, 132.7, 131.2, 129.2, 128.9, 128.4, 128.1, 125.7, 123.3, 122.7, 122.0, 121.9, 117.8, 110.4, 58.1, 52.4, 31.6, 23.8, 23.7, 21.1. HRMS (ESI) Calcd for $C_{36}H_{29}NNaO_4S^+$[M+Na]$^+$: 594.1715, Found: 594.1719.

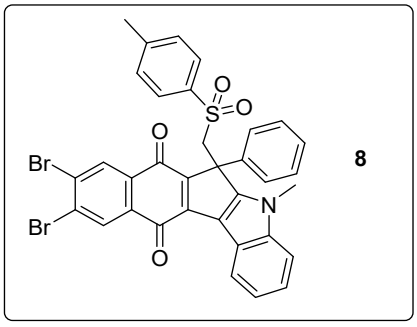
5,9,10-trimethyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (7)



7

Blue solid, m.p. 229-230 °C, yield: 48.0 mg, 42% yield; Rf: 0.34 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.4 (dt, *J* = 4.9, 2.3 Hz, 1H), 7.8 (s, 1H), 7.6 (s, 1H), 7.4 (d, *J* = 2.7 Hz, 3H), 7.2 (q, *J* = 4.3, 3.6 Hz, 5H), 7.1 (dd, *J* = 6.6, 3.2 Hz, 2H), 6.7 (d, *J* = 7.9 Hz, 2H), 5.5 (d, *J* = 14.5 Hz, 1H), 4.4 (d, *J* = 14.5 Hz, 1H), 3.6 (s, 3H), 2.4 (d, *J* = 6.5 Hz, 6H), 1.9 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.8, 179.2, 156.7, 145.0, 143.3, 142.9, 141.5, 136.3, 130.1, 129.2, 129.0, 128.5, 128.2, 127.0, 126.8, 125.7, 123.6, 122.7, 122.2, 121.8, 118.6, 110.5, 58.2, 52.4, 31.8, 21.1, 20.2, 19.9. HRMS (ESI) Calcd for $C_{36}H_{29}NNaO_4S^+$[M+Na]$^+$: 594.1715, Found: 594.1718.

9,10-dibromo-5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (8)

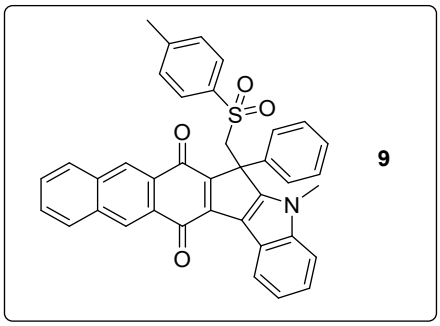


8

Blue solid, m.p. 295-296 °C, yield: 65.9 mg, 47% yield; Rf: 0.51 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.4 (dd, *J* = 6.2, 3.1 Hz, 1H), 8.2 (s, 1H), 8.1 (s, 1H), 7.4 – 7.4 (m, 3H), 7.2 (d, *J* = 6.8 Hz, 5H), 7.1 – 7.0 (m, 2H), 6.8 (d, *J* = 7.9 Hz, 2H), 5.4 (d, *J* = 14.6 Hz, 1H), 4.4 (d, *J* = 14.6 Hz, 1H), 3.6 (s, 3H), 2.0 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 181.0, 176.5, 157.8, 146.4, 145.2, 143.2, 142.1, 135.7, 134.7, 133.5, 131.6, 131.4, 131.2, 130.7, 129.6, 129.4, 129.2, 128.6, 128.6, 125.6, 124.1, 122.8, 122.7,

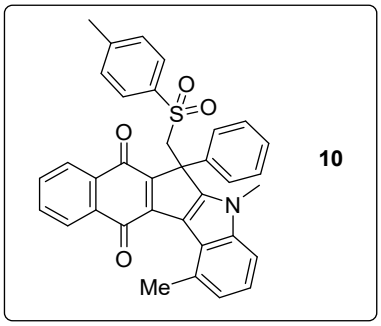
121.7, 118.2, 110.7, 58.2, 52.6, 31.9, 21.2. HRMS (ESI) Calcd for $C_{34}H_{23}Br_2NNaO_4S^+$[M+Na]$^+$: 721.9612, Found: 721.9614.

5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydronaphtho[2',3':5,6]indeno[2,1-*b*]indole-7,14-dione (9)



Blue solid, m.p. 271-272 °C, yield: 47.5 mg, 40% yield; Rf: 0.37 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.5 (d, *J* = 16.6 Hz, 2H), 8.3 (s, 1H), 8.0 – 7.9 (m, 2H), 7.7 – 7.6 (m, 2H), 7.4 (s, 3H), 7.2 (d, *J* = 8.8 Hz, 5H), 7.1 (dd, *J* = 6.8, 3.0 Hz, 2H), 6.7 (d, *J* = 7.8 Hz, 2H), 5.6 (d, *J* = 14.6 Hz, 1H), 4.4 (d, *J* = 14.6 Hz, 1H), 3.7 (s, 3H), 1.6 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.2, 178.3, 157.1, 147.9, 145.2, 144.0, 143.1, 136.3, 134.9, 134.3, 134.0, 130.8, 130.0, 129.9, 129.4, 129.3, 129.1, 129.0, 128.5, 128.4, 127.9, 127.7, 125.8, 123.8, 122.9, 122.4, 121.9, 118.6, 110.7, 58.3, 53.5, 52.6, 31.9, 21.0. HRMS (ESI) Calcd for $C_{38}H_{27}NNaO_4S^+$[M+Na]$^+$: 616.1558, Found: 616.1558.

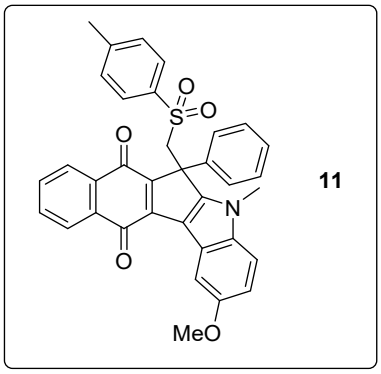
1,5-dimethyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (10)



Blue solid, m.p. 260-261 °C, yield: 56.9 mg, 51% yield; Rf: 0.40 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.95 (m, 1H), 7.86 – 7.79 (m, 1H), 7.67 – 7.55 (m, 2H), 7.29 (d, *J* = 8.5 Hz, 2H), 7.24 – 7.17 (m, 5H), 7.09 (dd, J = 6.7, 2.8 Hz, 2H), 6.74

(d, J = 7.9 Hz, 2H), 5.52 (d, *J* = 14.6 Hz, 1H), 4.40 (d, *J* = 14.7 Hz, 1H), 3.54 (s, 3H), 3.06 (s, 3H), 1.90 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) 182.5, 179.0, 157.6, 148.0, 145.2, 143.6, 143.2, 136.4, 134.6, 133.6, 133.3, 133.3, 133.1, 132.4, 129.3, 129.1, 128.4, 128.3, 126.0, 125.7, 125.3, 124.5, 123.6, 122.0, 116.6, 108.1, 58.0, 51.0, 31.7, 23.3, 21.3. HRMS (ESI) Calcd for $C_{35}H_{27}NNaO_4S^+$[M+Na]$^+$: 580.1558, Found: 580.1559.

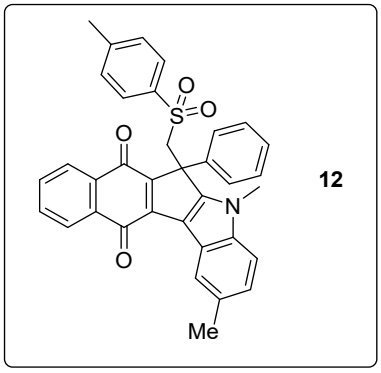
2-methoxy-5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (11)



11

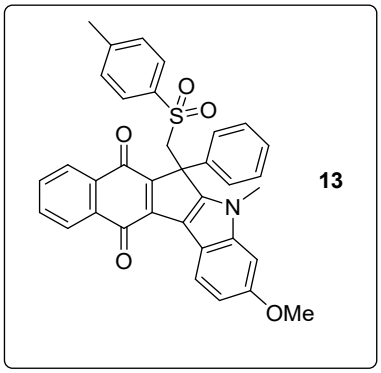
Blue solid, m.p. 323-324 ^{o}C, yield: 65.3 mg, 57% yield; Rf: 0.30 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.0 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.9 (d, *J* = 2.5 Hz, 1H), 7.9 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.6 (dtd, *J* = 19.5, 7.3, 1.6 Hz, 2H), 7.3 (d, *J* = 8.9 Hz, 1H), 7.3 – 7.2 (m, 6H), 7.1 (d, *J* = 3.4 Hz, 1H), 7.0 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.7 (d, *J* = 7.9 Hz, 2H), 5.5 (d, *J* = 14.6 Hz, 1H), 4.3 (d, *J* = 14.6 Hz, 1H), 4.1 (s, 3H), 3.6 (s, 3H), 1.9 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.9, 178.6, 157.1, 146.6, 145.3, 141.6, 138.0, 136.5, 134.4, 134.2, 133.7, 132.1, 132.1, 129.3, 129.1, 128.5, 128.3, 125.8, 125.7, 125.6, 122.4, 118.0, 113.7, 111.4, 104.4, 58.2, 56.0, 53.4, 52.4, 32.0, 21.2. HRMS (ESI) Calcd for $C_{35}H_{27}NNaO_5S^+$[M+Na]$^+$: 596.1508, Found: 596.1509.

2,5-dimethyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (12)



Blue solid, m.p. 308-309 °C, yield: 59.1 mg, 53% yield; Rf: 0.37 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.2 (s, 1H), 8.0 (dd, *J* = 7.3, 1.6 Hz, 1H), 7.9 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.7 – 7.6 (m, 2H), 7.3 (d, *J* = 8.4 Hz, 1H), 7.2 (dd, *J* = 9.0, 4.6 Hz, 5H), 7.1 – 7.0 (m, 3H), 6.7 (d, *J* = 8.0 Hz, 2H), 5.5 (d, *J* = 14.5 Hz, 1H), 4.4 (d, *J* = 14.5 Hz, 1H), 3.6 (s, 3H), 2.6 (s, 3H), 1.9 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.8, 178.5, 157.2, 146.6, 145.3, 141.8, 141.5, 136.4, 134.4, 134.2, 133.7, 132.1, 129.3, 129.1, 128.6, 128.3, 125.8, 125.7, 125.6, 125.3, 122.5, 121.9, 117.9, 110.3, 58.2, 52.4, 31.9, 21.6, 21.2. HRMS (ESI) Calcd for $C_{35}H_{27}NNaO_4S^+$[M+Na]$^+$: 580.1558, Found: 580.1560.

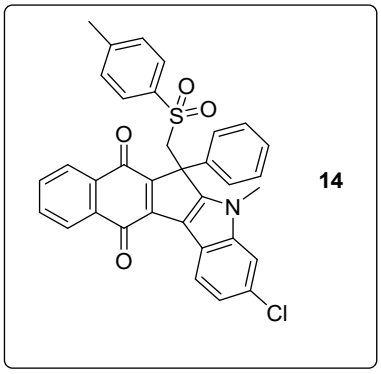
3-methoxy-5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (13)



Blue solid, m.p. 173-174 °C, yield: 59.7 mg, 52% yield; Rf: 0.23(EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.7 Hz, 1H), 8.00 (d, *J* = 7.5 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.69 – 7.55 (m, 2H), 7.21 (d, *J* = 8.4 Hz, 5H), 7.10 (d, *J* = 2.3 Hz, 2H), 7.05 (dd, *J* = 8.7, 2.1 Hz, 1H), 6.88 (s, 1H), 6.72 (d, *J* = 7.8 Hz, 2H), 5.48 (d, *J* = 14.5 Hz, 1H), 4.35 (d, *J* = 14.5 Hz, 1H), 3.95 (s, 3H), 3.60 (s, 3H), 1.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.8, 178.5, 157.7, 156.5, 146.3, 145.3, 144.1, 141.9, 136.5, 134.3,

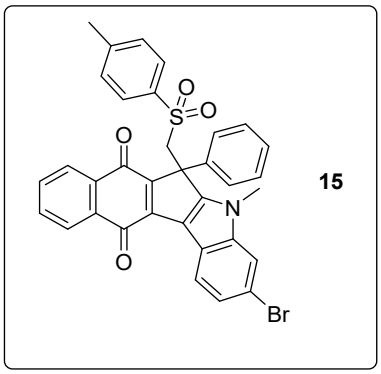
134.2, 133.7, 132.1, 132.1, 129.3, 129.0, 128.5, 128.3, 125.8, 125.7, 125.6, 123.5, 118.5, 115.8, 111.5, 94.8, 58.3, 55.8, 52.5, 32.0, 21.2. HRMS (ESI) Calcd for $C_{35}H_{27}NNaO_5S^+$[M+Na]$^+$: 596.1508, Found: 596.1508.

3-chloro-5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (14)



Purple solid, m.p. 305-306 °C, yield: 42.8 mg, 37% yield; Rf: 0.37 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.4 Hz, 1H), 8.02 (d, *J* = 7.2 Hz, 1H), 7.87 (d, *J* = 7.2 Hz, 1H), 7.64 (p, *J* = 7.2 Hz, 2H), 7.43 – 7.35 (m, 2H), 7.27 – 7.18 (m, 5H), 7.09 (s, 2H), 6.74 (d, *J* = 7.7 Hz, 2H), 5.46 (d, *J* = 14.6 Hz, 1H), 4.36 (d, *J* = 14.6 Hz, 1H), 3.60 (s, 3H), 1.89 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.5, 178.9, 157.3, 146.0, 145.4, 143.3, 142.9, 135.8, 134.4, 134.0, 133.8, 132.4, 132.0, 129.7, 129.4, 129.1, 128.5, 128.5, 125.9, 125.7, 125.6, 123.6, 122.9, 120.2, 118.2, 110.9, 58.2, 52.7, 32.0, 21.2. HRMS (ESI) Calcd for $C_{34}H_{24}ClNNaO_4S^+$[M+Na]$^+$: 600.1012, Found: 600.1010.

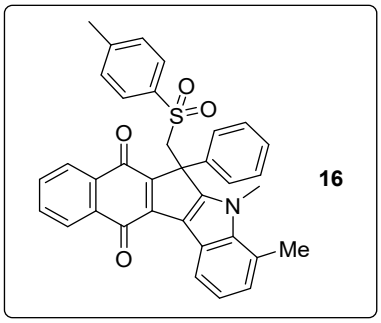
3-bromo-5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (15)



Purple solid, m.p. 310-311 °C, yield: 43.5 mg, 35% yield; Rf: 0.37 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.5 Hz, 1H), 8.02 (d, *J* = 7.3 Hz, 1H), 7.87 (d,

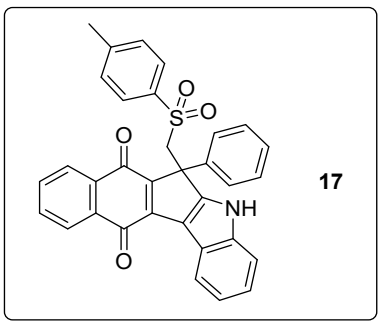
J = 7.4 Hz, 1H), 7.69 – 7.58 (m, 2H), 7.56 (s, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.22 (dd, *J* = 9.8, 5.8 Hz, 5H), 7.12 – 7.05 (m, 2H), 6.74 (d, *J* = 7.9 Hz, 2H), 5.46 (d, *J* = 14.6 Hz, 1H), 4.35 (d, *J* = 14.5 Hz, 1H), 3.60 (s, 3H), 1.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.5, 178.9, 157.2, 146.0, 145.4, 143.6, 143.0, 135.8, 134.3, 134.0, 133.8, 132.4, 132.0, 129.4, 129.1, 128.5, 128.5, 125.9, 125.7, 125.6, 125.6, 123.9, 120.5, 118.2, 117.3, 113.8, 58.1, 52.7, 32.0, 21.2. HRMS (ESI) Calcd for $C_{34}H_{24}BrNNaO_4S^+$[M+Na]$^+$: 644.0507, Found: 644.0510.

4,5-dimethyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (16)



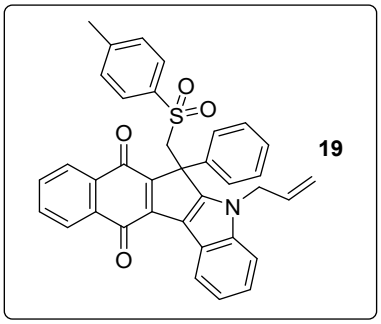
Blue solid, m.p. 285-286 °C, yield: 66.8 mg, 60% yield; Rf: 0.34 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 7.9 Hz, 1H), 7.87 (d, *J* = 8.2 Hz, 1H), 7.69 – 7.56 (m, 2H), 7.29 – 7.19 (m, 6H), 7.10 (t, *J* = 7.3 Hz, 3H), 6.72 (d, *J* = 7.9 Hz, 2H), 5.50 (d, *J* = 14.5 Hz, 1H), 4.37 (d, *J* = 14.5 Hz, 1H), 3.81 (s, 3H), 2.77 (s, 3H), 1.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.7, 178.7, 157.3, 146.4, 145.2, 142.4, 141.4, 136.2, 134.5, 134.1, 133.7, 132.2, 132.1, 129.3, 129.1, 128.5, 128.3, 127.1, 125.8, 125.7, 122.7, 122.5, 121.0, 118.4, 58.2, 53.4, 52.6, 35.8, 21.2, 19.8. HRMS (ESI) Calcd for $C_{35}H_{27}NNaO_4S^+$[M+Na]$^+$: 580.1558, Found: 580.1562.

6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (17)



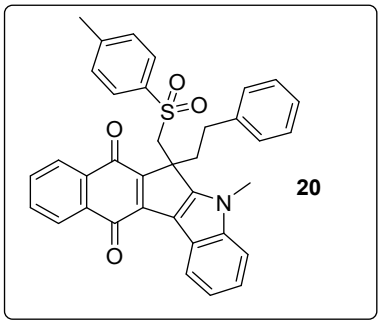
Blue solid, m.p. 271-272 °C, yield: 45.5 mg, 43% yield; Rf: 0.23 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.91 (s, 1H), 8.50 – 8.44 (m, 1H), 8.09 (dd, *J* = 7.3, 1.8 Hz, 1H), 7.99 – 7.92 (m, 1H), 7.70 – 7.59 (m, 2H), 7.56 – 7.49 (m, 1H), 7.38 (d, *J* = 8.1 Hz, 4H), 7.14 (dq, *J* = 23.4, 7.8, 6.8 Hz, 5H), 7.00 (d, *J* = 7.9 Hz, 2H), 5.07 (d, *J* = 15.0 Hz, 1H), 4.32 (d, *J* = 15.0 Hz, 1H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 183.0, 179.3, 156.4, 146.2, 145.1, 142.9, 141.8, 136.3, 135.3, 134.1, 133.9, 132.5, 132.1, 129.5, 128.7, 128.0, 127.0, 126.1, 125.9, 124.2, 122.7, 122.4, 121.7, 119.2, 113.0, 59.7, 54.3, 21.4. HRMS (ESI) Calcd for $C_{33}H_{23}NNaO_4S^+$[M+Na]$^+$: 552.1245, Found: 552.1246.

5-allyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (19)



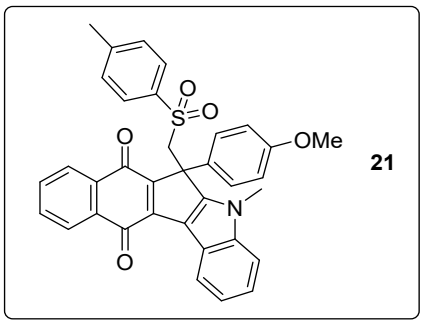
Blue solid, m.p. 231-232 °C, yield: 63.7 mg, 56% yield; Rf: 0.34 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.7 Hz, 1H), 8.05 (d, *J* = 9.0 Hz, 1H), 7.82 (d, *J* = 7.0 Hz, 1H), 7.68 – 7.57 (m, 2H), 7.43 – 7.33 (m, 3H), 7.27 – 7.18 (m, 5H), 7.06 (dd, *J* = 6.6, 3.1 Hz, 2H), 6.75 (d, *J* = 7.8 Hz, 2H), 5.63 (ddt, *J* = 16.5, 10.4, 6.0 Hz, 1H), 5.42 (d, *J* = 14.5 Hz, 1H), 5.19 – 5.03 (m, 2H), 4.69 – 4.52 (m, 2H), 4.44 (d, *J* = 14.6 Hz, 1H), 1.89 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.7, 178.6, 157.4, 146.6, 145.2, 143.0, 142.5, 136.3, 134.6, 134.0, 133.7, 132.2, 132.2, 131.9, 129.3, 129.2, 129.1, 128.5, 128.4, 128.3, 125.8, 125.7, 125.5, 125.3, 123.7, 122.8, 122.4, 122.2, 122.0, 118.8, 118.3, 111.8, 57.8, 52.3, 49.1, 21.2. HRMS (ESI) Calcd for $C_{36}H_{27}NNaO_4S^+$[M+Na]$^+$: 592.1558, Found: 592.1562.

5-methyl-6-phenethyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (20)



Blue solid, m.p. 89-90 °C, yield: 26.3 mg, 23% yield; Rf: 0.34 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (dd, *J* = 7.0, 2.7 Hz, 1H), 8.06 (d, *J* = 7.5 Hz, 1H), 7.96 (d, *J* = 7.6 Hz, 1H), 7.72 (t, *J* = 7.4 Hz, 1H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.39 (q, *J* = 4.8 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 6.97 (q, *J* = 7.9, 7.3 Hz, 3H), 6.70 (dd, *J* = 15.7, 7.4 Hz, 4H), 4.89 (d, *J* = 15.0 Hz, 1H), 3.92 (d, *J* = 15.0 Hz, 1H), 3.82 (s, 3H), 2.92 (ddd, *J* = 14.2, 9.5, 6.5 Hz, 1H), 2.43 (ddd, *J* = 13.9, 9.6, 6.4 Hz, 1H), 2.12 (dt, *J* = 15.4, 8.8 Hz, 1H), 1.86 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.2, 179.2, 155.6, 147.8, 145.2, 143.2, 140.0, 139.1, 134.5, 134.2, 133.7, 132.2, 129.1, 128.4, 128.2, 128.1, 126.0, 125.8, 125.7, 123.6, 122.6, 122.3, 121.7, 118.7, 110.4, 59.6, 50.5, 38.4, 31.9, 29.5, 21.2. HRMS (ESI) Calcd for $C_{36}H_{29}NNaO_4S^+$[M+Na]$^+$:594.1715, Found: 594.1719.

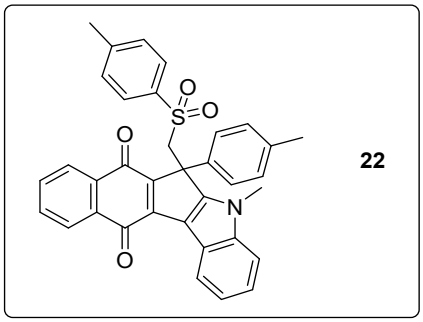
6-(4-methoxyphenyl)-5-methyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (21)



Blue solid, m.p. 246-247 °C, yield: 80.2 mg, 70% yield; Rf: 0.31 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 3.5 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 6.8 Hz, 1H), 7.69 – 7.56 (m, 2H), 7.41 (d, *J* = 3.2 Hz, 3H), 7.20 (d, *J* = 7.9 Hz, 2H), 7.02 (d, *J* = 8.5 Hz, 2H), 6.72 (t, *J* = 7.4 Hz, 4H), 5.46 (d, *J* = 14.5 Hz, 1H), 4.34 (d, *J* = 14.5 Hz, 1H), 3.71 (s, 3H), 3.65 (s, 3H), 1.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.7, 178.8, 159.4, 157.0, 146.2, 145.3, 143.0, 142.3, 134.3, 134.1, 133.7, 132.2, 132.1, 129.0, 128.5, 127.7, 126.9, 125.8, 125.6, 123.7, 122.7, 122.3, 121.7, 118.0,

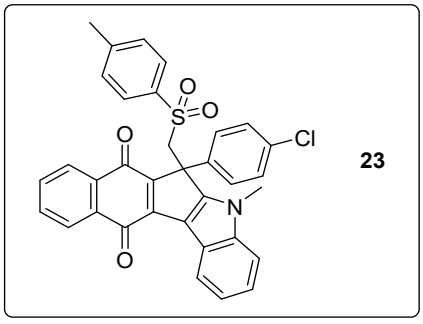
114.6, 110.6, 58.4, 55.2, 52.0, 31.9, 21.2. HRMS (ESI) Calcd for $C_{35}H_{27}NNaO_5S^+$[M+Na]$^+$: 596.1508, Found: 596.1509.

5-methyl-6-(*p*-tolyl)-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (22)



Blue solid, m.p. 244-245 °C, yield: 70.2 mg, 63% yield; Rf: 0.49 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (dq, *J* = 5.4, 2.1 Hz, 1H), 8.02 (dd, *J* = 7.2, 1.7 Hz, 1H), 7.86 (dd, *J* = 7.3, 1.7 Hz, 1H), 7.68 – 7.55 (m, 2H), 7.41 (d, *J* = 2.8 Hz, 3H), 7.21 (d, *J* = 8.3 Hz, 2H), 7.00 (q, *J* = 8.5 Hz, 4H), 6.72 (d, *J* = 8.0 Hz, 2H), 5.47 (d, *J* = 14.6 Hz, 1H), 4.35 (d, *J* = 14.6 Hz, 1H), 3.64 (s, 3H), 2.23 (s, 3H), 1.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.7, 178.7, 157.1, 146.4, 145.3, 143.0, 142.3, 138.3, 134.4, 134.1, 133.6, 133.0, 132.2, 132.1, 130.0, 129.1, 128.5, 125.8, 125.6, 125.5, 123.7, 122.7, 122.3, 121.8, 118.2, 110.6, 77.4, 77.0, 76.7, 58.3, 52.2, 31.9, 21.2, 20.9. HRMS (ESI) Calcd for $C_{35}H_{27}NNaO_4S^+$[M+Na]$^+$: 580.1558, Found: 580.1560.

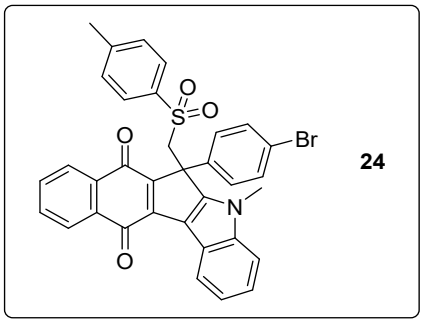
6-(4-chlorophenyl)-5-methyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (23)



Blue solid, m.p. 210-211 °C, yield: 81.9 mg, 71% yield; Rf: 0.49 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 – 8.41 (m, 1H), 8.03 (dd, *J* = 7.2, 1.7 Hz, 1H), 7.86 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.70 – 7.57 (m, 2H), 7.42 (d, *J* = 2.8 Hz, 3H), 7.19 (dd, *J* = 8.6, 6.8 Hz, 4H), 7.08 – 7.00 (m, 2H), 6.72 (d, *J* = 8.1 Hz, 2H), 5.43 (d, *J* = 14.5 Hz,

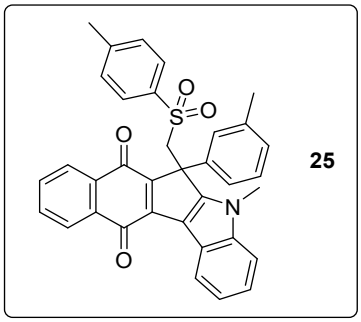
1H), 4.33 (d, *J* = 14.5 Hz, 1H), 3.64 (s, 3H), 1.88 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.5, 178.7, 156.5, 146.5, 145.4, 143.0, 141.8, 134.9, 134.3, 134.2, 134.0, 133.8, 132.3, 132.1, 129.4, 129.1, 128.5, 127.2, 125.8, 125.7, 123.9, 122.8, 122.5, 121.7, 118.4, 110.7, 58.0, 52.0, 31.9, 21.2. HRMS (ESI) Calcd for $C_{34}H_{24}ClNNaO_4S^+$[M+Na]$^+$: 600.1012, Found: 600.1014.

6-(4-bromophenyl)-5-methyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (24)



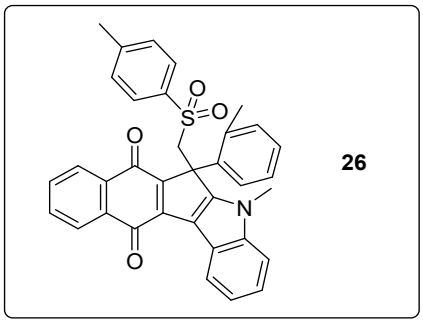
Blue solid, m.p. 143-144 °C, yield: 109.3 mg, 88% yield; Rf: 0.51 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (dp, *J* = 6.1, 1.8 Hz, 1H), 8.06 – 8.00 (m, 1H), 7.89 – 7.83 (m, 1H), 7.63 (dtd, *J* = 16.6, 7.4, 1.5 Hz, 2H), 7.47 – 7.39 (m, 3H), 7.37 – 7.29 (m, 2H), 7.20 (d, *J* = 8.3 Hz, 2H), 7.01 – 6.93 (m, 2H), 6.72 (d, *J* = 8.6 Hz, 2H), 5.42 (d, *J* = 14.5 Hz, 1H), 4.32 (d, *J* = 14.5 Hz, 1H), 3.64 (s, 3H), 1.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.5, 178.7, 156.4, 146.5, 145.4, 143.0, 141.7, 135.4, 134.2, 134.0, 133.8, 132.4, 132.3, 132.0, 129.1, 128.5, 127.5, 125.8, 125.7, 123.9, 122.8, 122.5, 122.5, 121.7, 118.4, 110.7, 57.9, 52.0, 31.9, 21.2. HRMS (ESI) Calcd for $C_{34}H_{24}BrNNaO_4S^+$[M+Na]$^+$: 644.0507, Found: 644.0510.

5-methyl-6-(*m*-tolyl)-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (25)



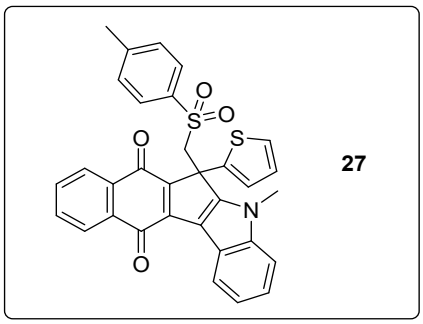
Blue solid, m.p. 141-142 °C, yield: 59.1 mg, 53% yield; Rf: 0.46 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (dt, *J* = 4.9, 2.2 Hz, 1H), 8.03 (d, *J* = 7.3 Hz, 1H), 7.86 (d, *J* = 7.4 Hz, 1H), 7.68 – 7.58 (m, 2H), 7.41 (s, 3H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.10 (t, *J* = 7.8 Hz, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.93 (s, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 6.72 (d, *J* = 7.9 Hz, 2H), 5.46 (d, *J* = 14.5 Hz, 1H), 4.38 (d, *J* = 14.5 Hz, 1H), 3.64 (s, 3H), 2.23 (s, 3H), 1.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.7, 178.6, 157.2, 146.6, 145.2, 143.0, 142.3, 139.0, 135.9, 134.4, 134.1, 133.6, 132.1, 132.1, 129.2, 129.1, 129.0, 128.5, 126.2, 125.8, 125.6, 123.6, 122.7, 122.6, 122.3, 121.8, 118.1, 110.6, 58.2, 52.3, 31.8, 21.6, 21.2. HRMS (ESI) Calcd for $C_{35}H_{27}NNaO_4S^+$[M+Na]$^+$: 580.1558, Found: 580.1561.

5-methyl-6-(*o*-tolyl)-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (26)



Blue solid, m.p. 247-248 °C, yield: 54.6 mg, 49% yield; Rf: 0.40 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 8.6 Hz, 1H), 8.06 (d, *J* = 8.8 Hz, 1H), 7.88 (d, *J* = 7.1 Hz, 1H), 7.80 (d, *J* = 8.2 Hz, 1H), 7.65 (p, *J* = 7.3, 6.8 Hz, 2H), 7.39 (p, *J* = 7.1 Hz, 3H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 7.7 Hz, 3H), 6.90 (d, *J* = 7.5 Hz, 1H), 6.74 (d, *J* = 7.9 Hz, 2H), 5.26 (d, *J* = 14.1 Hz, 1H), 4.54 (d, *J* = 14.1 Hz, 1H), 3.49 (s, 3H), 1.95 (s, 3H), 1.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 181.8, 177.9, 156.2, 147.0, 143.7, 141.5, 137.7, 135.5, 134.1, 133.1, 132.7, 132.1, 132.0, 131.3, 131.2, 128.2, 127.2, 126.8, 126.6, 126.2, 124.9, 124.7, 122.7, 121.8, 121.5, 121.0, 118.2, 109.6, 58.6, 50.6, 30.2, 20.3, 18.5. HRMS (ESI) Calcd for $C_{35}H_{27}NNaO_4S^+$[M+Na]$^+$: 580.1558, Found: 580.1561.

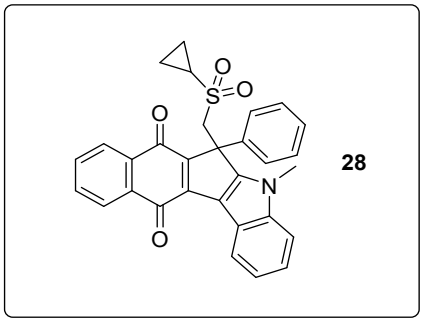
5-methyl-6-(thiophen-2-yl)-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (27)



27

Blue solid, m.p. 247-248 °C, yield: 27.5 mg, 25% yield; Rf: 0.37 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 – 8.39 (m, 1H), 8.03 (d, *J* = 7.5 Hz, 1H), 7.91 (d, *J* = 7.5 Hz, 1H), 7.65 (dt, *J* = 21.4, 7.4 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 3H), 7.20 (d, *J* = 7.9 Hz, 2H), 7.10 (d, *J* = 6.2 Hz, 1H), 7.02 (d, *J* = 3.8 Hz, 1H), 6.88 (t, *J* = 4.5 Hz, 1H), 6.72 (d, *J* = 7.9 Hz, 2H), 5.48 (d, *J* = 14.7 Hz, 1H), 4.36 (d, *J* = 14.7 Hz, 1H), 3.80 (s, 3H), 1.85 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.6, 178.7, 155.7, 145.9, 145.4, 143.0, 140.6, 139.0, 134.1, 134.0, 133.7, 132.3, 132.0, 129.1, 128.6, 127.1, 125.8, 125.7, 125.7, 125.0, 123.9, 122.9, 122.5, 121.7, 117.6, 110.7, 59.1, 50.3, 32.2, 21.2. HRMS (ESI) Calcd for $C_{32}H_{23}NNaO_4S_2^+$[M+Na]$^+$: 572.0966, Found: 572.0969.

6-((cyclopropylsulfonyl)methyl)-5-methyl-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (28)

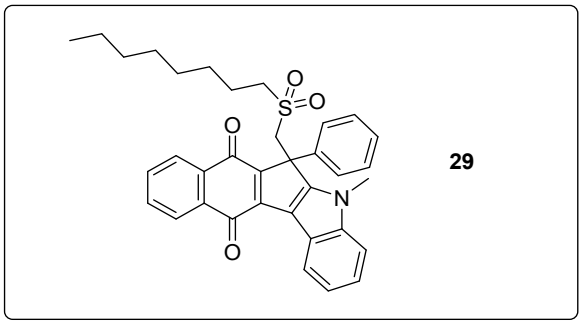


28

Blue solid, m.p. 283-284 °C, yield: 34.5 mg, 35% yield; Rf: 0.17 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 – 8.44 (m, 1H), 8.15 (dd, *J* = 7.3, 1.6 Hz, 1H), 8.08 – 7.98 (m, 1H), 7.66 (pd, *J* = 7.4, 1.7 Hz, 2H), 7.46 – 7.33 (m, 3H), 7.31 – 7.21 (m, 3H), 7.17 (dd, *J* = 6.8, 3.1 Hz, 2H), 5.40 (d, *J* = 14.1 Hz, 1H), 4.30 (d, *J* = 14.1 Hz, 1H), 3.68 (s, 3H), 2.10 (tt, *J* = 7.9, 4.8 Hz, 1H), 1.12 – 0.97 (m, 2H), 0.82 – 0.67 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) 183.2, 179.4, 157.8, 146.6, 143.9, 143.0, 136.0, 134.2, 134.0, 132.6, 132.4, 129.4, 128.5, 126.3, 126.1, 125.8, 123.8, 123.1, 122.5, 122.0, 118.1,

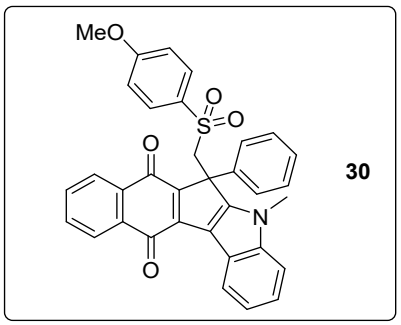
110.5, 57.1, 52.4, 31.8, 30.5, 5.3, 5.2. HRMS (ESI) Calcd for $C_{30}H_{23}NNaO_4S^+[M+Na]^+$: 516.1245, Found: 516.1249.

5-methyl-6-((octylsulfonyl)methyl)-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (29)



Blue solid, m.p. 127-128 °C, yield: 37.3 mg, 33% yield; Rf: 0.71 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (ddd, *J* = 6.6, 3.3, 2.2 Hz, 1H), 8.20 – 8.11 (m, 1H), 8.06 – 7.98 (m, 1H), 7.73 – 7.60 (m, 2H), 7.46 – 7.33 (m, 3H), 7.26 (d, *J* = 6.6 Hz, 3H), 7.20 – 7.11 (m, 2H), 5.35 – 5.27 (m, 1H), 4.19 (d, *J* = 14.0 Hz, 1H), 3.68 (s, 3H), 2.76 (t, *J* = 8.1 Hz, 2H), 1.68 (pd, *J* = 8.0, 4.1 Hz, 2H), 1.41 – 1.17 (m, 3H), 1.11 (t, *J* = 6.0 Hz, 7H), 0.84 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 183.1, 179.4, 157.8, 146.7, 143.4, 143.0, 136.1, 134.1, 133.9, 132.6, 132.5, 129.4, 128.4, 126.3, 126.1, 125.7, 123.8, 123.1, 122.5, 122.0, 118.2, 110.5, 55.6, 54.4, 52.1, 31.9, 31.6, 28.8, 28.8, 28.3, 22.5, 21.8, 14.0. HRMS (ESI) Calcd for $C_{35}H_{35}NNaO_4S^+[M+Na]^+$: 588.2184, Found: 588.2188.

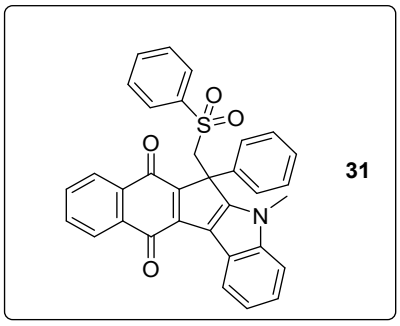
6-(((4-methoxyphenyl)sulfonyl)methyl)-5-methyl-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (30)



Blue solid, m.p. 255-256 °C, yield: 71.6 mg, 64% yield; Rf: 0.28 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 – 8.42 (m, 1H), 8.06 – 7.99 (m, 1H), 7.91 – 7.84 (m, 1H), 7.63 (pd, *J* = 7.4, 1.6 Hz, 2H), 7.46 – 7.39 (m, 3H), 7.26 – 7.18 (m, 5H), 7.15 –

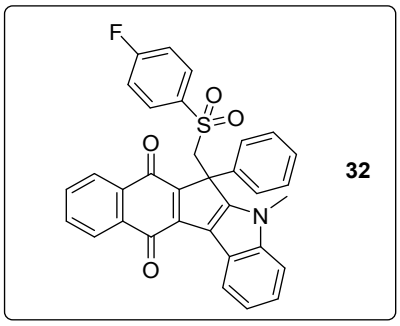
7.05 (m, 2H), 6.40 – 6.32 (m, 2H), 5.48 (d, *J* = 14.6 Hz, 1H), 4.37 (d, *J* = 14.5 Hz, 1H), 3.64 (s, 3H), 3.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.8, 178.7, 163.6, 157.0, 146.4, 143.0, 142.3, 136.2, 134.1, 133.7, 132.2, 132.1, 130.7, 129.3, 128.5, 128.3, 125.8, 125.7, 123.7, 122.7, 122.4, 121.7, 118.3, 113.5, 112.1, 110.6, 58.5, 55.2, 52.5, 31.9. HRMS (ESI) Calcd for $C_{34}H_{25}NNaO_5S$ $^+$[M+Na]$^+$: 582.1351, Found: 582.1355.

5-methyl-6-phenyl-6-((phenylsulfonyl)methyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (31)



Blue solid, m.p. 277-278 °C, yield: 84.66 mg, 80% yield; Rf: 0.57 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 – 8.42 (m, 1H), 8.06 – 7.96 (m, 1H), 7.91 – 7.82 (m, 1H), 7.66 – 7.58 (m, 2H), 7.44 – 7.35 (m, 5H), 7.22 (dp, *J* = 5.9, 2.2 Hz, 3H), 7.14 – 7.07 (m, 2H), 7.07 – 7.01 (m, 1H), 7.01 – 6.93 (m, 2H), 5.51 (d, *J* = 14.6 Hz, 1H), 4.40 (d, *J* = 14.5 Hz, 1H), 3.58 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.9, 178.9, 156.9, 146.5, 142.9, 142.3, 137.7, 136.1, 134.0, 133.7, 133.6, 132.4, 132.2, 129.3, 128.4, 128.3, 125.8, 125.8, 125.7, 123.7, 122.8, 122.4, 121.8, 118.3, 110.6, 58.1, 52.4, 31.8. HRMS (ESI) Calcd for $C_{33}H_{23}NNaO_4S^+$[M+Na]$^+$: 552.1245, Found: 552.1248.

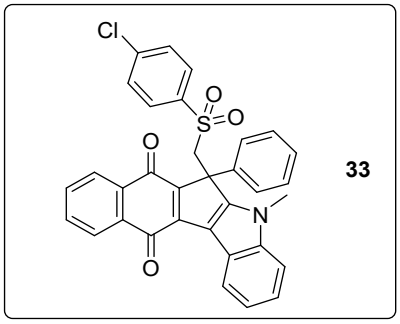
6-(((4-fluorophenyl)sulfonyl)methyl)-5-methyl-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (32)



Blue solid, m.p. 270-271 °C, yield: 56.9 mg, 52% yield; Rf: 0.40 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 – 8.43 (m, 1H), 8.10 – 8.01 (m, 1H), 7.92 – 7.82 (m,

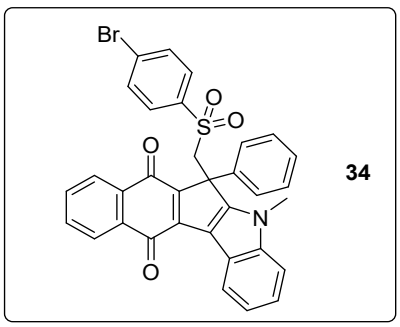
1H), 7.71 – 7.59 (m, 2H), 7.45 – 7.35 (m, 5H), 7.25 – 7.18 (m, 3H), 7.11 (dt, *J* = 5.6, 4.0 Hz, 2H), 6.67 – 6.57 (m, 2H), 5.50 (d, *J* = 14.6 Hz, 1H), 4.40 (d, *J* = 14.6 Hz, 1H), 3.61 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.8, 178.9, 167.0, 164.4, 157.0, 146.6, 143.0, 142.2, 135.9, 133.9, 133.9, 133.7, 133.7, 132.6, 132.0, 131.4, 131.3, 129.4, 128.5, 126.0, 125.8, 125.6, 123.9, 122.9, 122.6, 121.7, 118.3, 115.8, 115.6, 110.6, 77.4, 77.0, 76.7, 58.3, 52.4, 31.8. ^{19}F NMR (376 MHz, $CDCl_3$) -102.4. HRMS (ESI) Calcd for $C_{33}H_{22}FNNaO_4S^+$[M+Na]$^+$: 570.1151, Found: 570.1155.

6-(((4-chlorophenyl)sulfonyl)methyl)-5-methyl-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (33)



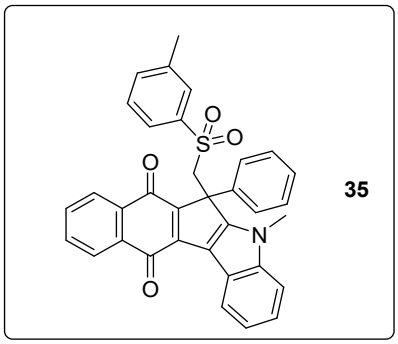
Blue solid, m.p. 225-226 °C, yield: 66.44 mg, 59% yield; Rf: 0.46 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.08 (d, *J* = 7.2 Hz, 1H), 7.86 (d, *J* = 7.2 Hz, 1H), 7.64 (q, *J* = 7.5 Hz, 2H), 7.43 (d, *J* = 10.4 Hz, 3H), 7.29 (s, 1H), 7.28 – 7.22 (m, 4H), 7.14 – 7.07 (m, 2H), 6.90 (d, *J* = 8.1 Hz, 2H), 5.50 (d, *J* = 14.6 Hz, 1H), 4.40 (d, *J* = 14.6 Hz, 1H), 3.62 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.7, 178.9, 156.9, 146.7, 143.0, 142.1, 141.0, 135.9, 135.9, 134.0, 133.8, 132.6, 132.0, 129.8, 129.4, 128.8, 128.5, 126.2, 125.7, 125.6, 124.0, 122.9, 122.6, 121.7, 118.3, 110.7, 58.3, 52.4, 31.9. HRMS (ESI) Calcd for $C_{33}H_{22}ClNNaO_4S^+$[M+Na]$^+$: 586.0856, Found: 586.0855.

6-(((4-bromophenyl)sulfonyl)methyl)-5-methyl-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (34)



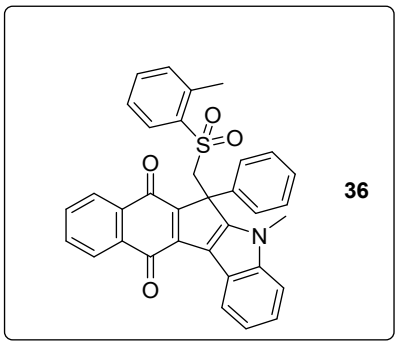
Blue solid, m.p. 233-234 °C, yield: 63.1 mg, 52% yield; Rf: 0.46 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (t, *J* = 3.7 Hz, 1H), 8.10 (d, *J* = 5.8 Hz, 1H), 7.87 (d, *J* = 8.9 Hz, 1H), 7.73 – 7.60 (m, 2H), 7.43 (d, *J* = 3.3 Hz, 3H), 7.26 – 7.16 (m, 5H), 7.15 – 7.05 (m, 4H), 5.51 (d, *J* = 14.6 Hz, 1H), 4.39 (d, *J* = 14.6 Hz, 1H), 3.63 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.7, 178.9, 156.9, 146.7, 143.0, 142.1, 136.4, 135.9, 134.0, 133.8, 132.7, 132.0, 131.8, 129.8, 129.8, 129.4, 128.5, 126.3, 125.7, 125.6, 124.0, 122.9, 122.6, 121.7, 118.3, 110.7, 58.2, 52.4, 31.9. HRMS (ESI) Calcd for $C_{33}H_{22}BrNNaO_4S^+$[M+Na]$^+$: 630.0351, Found: 630.0352.

5-methyl-6-phenyl-6-((m-tolylsulfonyl)methyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (35)



Blue solid, m.p. 282-283°C, yield: 63.0 mg, 58% yield; Rf: 0.39 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 – 8.43 (m, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.88 (d, *J* = 6.6 Hz, 1H), 7.68 – 7.57 (m, 2H), 7.41 (d, *J* = 3.8 Hz, 3H), 7.28 – 7.16 (m, 4H), 7.15 – 7.05 (m, 3H), 6.84 (t, *J* = 7.6 Hz, 1H), 6.79 (d, *J* = 7.7 Hz, 1H), 5.50 (d, *J* = 14.5 Hz, 1H), 4.39 (d, *J* = 14.6 Hz, 1H), 3.59 (s, 3H), 1.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.6, 178.9, 156.9, 146.4, 143.0, 142.3, 139.1, 137.4, 136.2, 134.6, 134.0, 133.6, 132.4, 132.2, 129.3, 129.0, 128.4, 128.3, 125.8, 125.7, 125.7, 123.8, 122.9, 122.4, 121.8, 118.4, 110.7, 58.1, 52.4, 31.8, 20.7. HRMS (ESI) Calcd for $C_{34}H_{25}NNaO_4S^+$[M+Na]$^+$: 566.1402, Found: 566.1407.

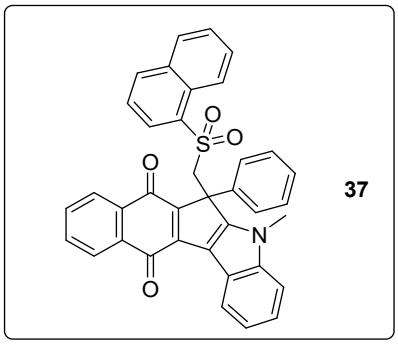
5-methyl-6-phenyl-6-((o-tolylsulfonyl)methyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (36)



36

Blue solid, m.p. 280-281 °C, yield: 57.6 mg, 53% yield; Rf: 0.41 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 – 8.41 (m, 1H), 8.01 – 7.94 (m, 1H), 7.89 – 7.81 (m, 1H), 7.60 (tt, *J* = 7.4, 5.6 Hz, 2H), 7.41 (d, *J* = 3.4 Hz, 3H), 7.24 – 7.19 (m, 3H), 7.15 – 7.08 (m, 3H), 6.86 – 6.76 (m, 2H), 6.67 (d, *J* = 6.7 Hz, 1H), 5.51 (d, *J* = 14.6 Hz, 1H), 4.37 (d, *J* = 14.5 Hz, 1H), 3.66 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 182.9, 178.5, 157.6, 146.5, 143.1, 142.1, 138.7, 136.3, 135.9, 134.0, 133.7, 133.6, 132.3, 132.2, 132.2, 130.8, 129.3, 128.4, 125.9, 125.7, 125.7, 125.6, 123.7, 122.8, 122.4, 121.8, 118.3, 110.7, 77.4, 77.1, 76.8, 56.8, 52.4, 31.9, 20.2. HRMS (ESI) Calcd for $C_{34}H_{25}NNaO_4S^+$[M+Na]$^+$: 566.1402, Found: 566.1407.

5-methyl-6-((naphthalen-1-ylsulfonyl)methyl)-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (37)

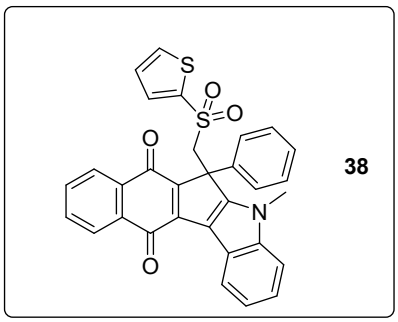


37

Blue solid, m.p. 282-283 °C, yield: 93.8mg, 81% yield; Rf: 0.46 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 8.7 Hz, 1H), 8.46 – 8.36 (m, 1H), 7.90 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.62 – 7.34 (m, 8H), 7.30 – 7.24 (m, 3H), 7.21 – 7.16 (m, 3H), 7.07 (dt, *J* = 5.5, 4.0 Hz, 2H), 7.01 – 6.92 (m, 1H), 5.66 (d, *J* = 14.5 Hz, 1H), 4.57 (d, *J* = 14.5 Hz, 1H), 3.50 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) 182.6, 178.0, 156.3, 145.7, 142.9, 142.6, 136.3, 135.7, 133.4, 133.2, 133.1, 132.1, 132.0, 131.9, 131.5, 129.2,

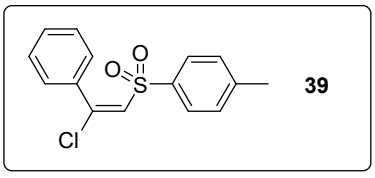
128.8, 128.6, 128.5, 128.3, 126.8, 125.9, 125.7, 125.4, 123.9, 123.8, 123.7, 122.7, 122.4, 121.6, 118.7, 110.6, 57.8, 52.3, 31.9. HRMS (ESI) Calcd for $C_{37}H_{25}NNaO_4S^+[M+Na]^+$: 602.1402, Found: 602.1406.

5-methyl-6-phenyl-6-((thiophen-2-ylsulfonyl)methyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (38)



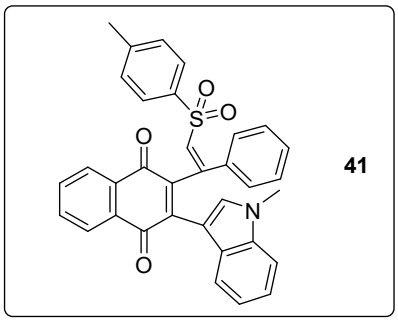
Blue solid, m.p. 239-240 °C, yield: 88.8 mg, 83% yield; Rf: 0.31 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (dt, *J* = 5.8, 2.9 Hz, 1H), 8.07 (dd, *J* = 7.2, 1.8 Hz, 1H), 7.98 – 7.89 (m, 1H), 7.70 – 7.58 (m, 2H), 7.46 – 7.34 (m, 3H), 7.25 – 7.17 (m, 4H), 7.12 (dd, *J* = 6.7, 3.1 Hz, 2H), 7.08 (d, *J* = 3.8 Hz, 1H), 6.58 – 6.52 (m, 1H), 5.57 (d, *J* = 14.6 Hz, 1H), 4.50 (d, *J* = 14.6 Hz, 1H), 3.57 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 183.0, 179.0, 156.6, 146.6, 142.9, 142.7, 139.0, 136.0, 135.1, 134.2, 134.1, 133.8, 132.4, 132.3, 129.4, 128.4, 127.5, 125.9, 125.9, 125.7, 123.7, 122.9, 122.4, 121.8, 118.5, 110.5, 59.8, 52.6, 31.7. HRMS (ESI) Calcd for $C_{31}H_{21}NNaO_4S_2^+[M+Na]^+$: 558.0810, Found: 558.0812.

(*E*)-1-((2-chloro-2-phenylvinyl)sulfonyl)-4-methylbenzene (39)



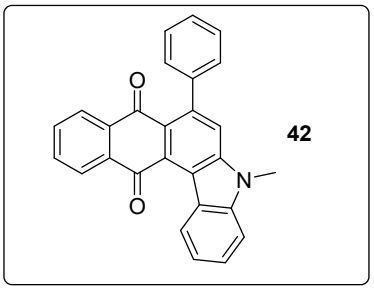
White solid, m.p. 118-119 °C, yield: 5.2 mg, 9% yield; Rf: 0.26 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.90 (m, 2H), 7.64 – 7.56 (m, 2H), 7.50 – 7.43 (m, 1H), 7.43 – 7.33 (m, 4H), 7.12 (s, 1H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 146.0, 144.9, 137.9, 135.3, 131.6, 129.8, 129.1, 128.8, 128.3, 128.0, 127.7, 127.2, 21.7.

2-(1-methyl-1*H*-indol-3-yl)-3-(1-phenyl-2-tosylvinyl)naphthalene-1,4-dione (41)



Purple solid, m.p. 139-140 °C, yield: 15.2 mg, 14% yield; Rf: 0.26 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (t, *J* = 6.4 Hz, 2H), 7.80 – 7.70 (m, 2H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.32 – 7.23 (m, 3H), 7.15 – 7.10 (m, 1H), 7.05 (d, *J* = 8.3 Hz, 3H), 6.99 (d, *J* = 7.4 Hz, 1H), 6.89 – 6.79 (m, 3H), 6.62 (d, *J* = 6.8 Hz, 2H), 3.76 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 184.6, 182.6, 146.6, 143.7, 142.5, 141.8, 138.1, 136.7, 135.7, 134.7, 134.0, 133.8, 132.4, 132.1, 132.1, 129.2, 128.8, 128.3, 127.6, 127.3, 126.8, 126.7, 122.6, 121.0, 120.8, 109.6, 107.5, 33.2, 21.5. HRMS (ESI) Calcd for $C_{34}H_{26}NO_4S^+[M+H]^+$: 544.1583, Found: 544.1583.

5-methyl-7-phenyl-5H-naphtho[2,3-*c*]carbazole-8,13-dione (42)

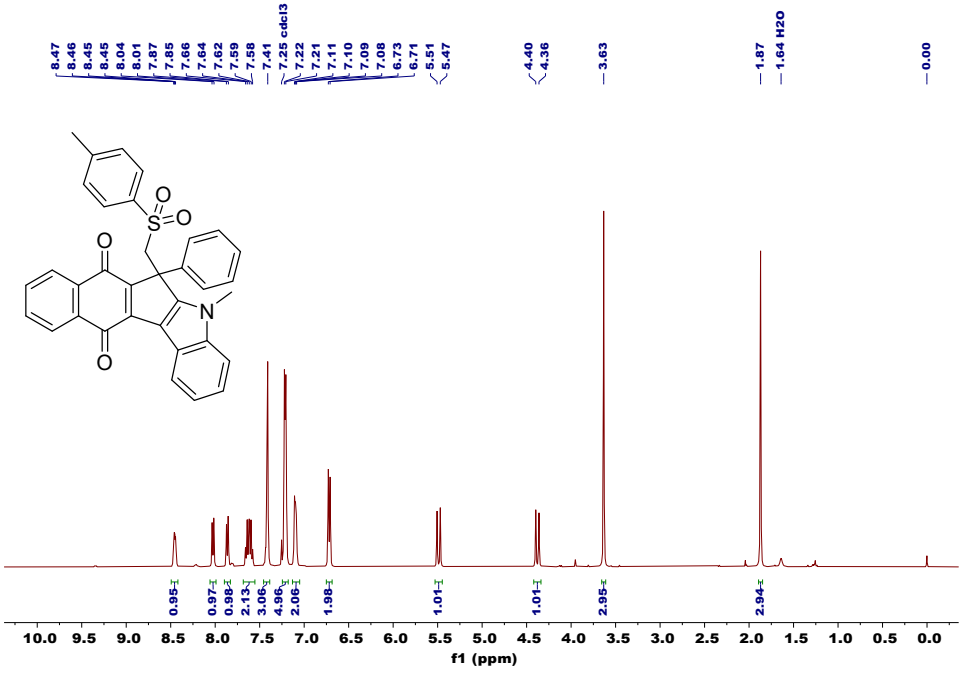


Yellow solid, m.p. 279-280 °C, yield: 1.5 mg, 2% yield; Rf: 0.71 (EA:PE =1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.45 (d, *J* = 8.3 Hz, 1H), 8.33 (d, *J* = 7.5 Hz, 1H), 8.11 – 8.05 (m, 1H), 7.72 (ddd, *J* = 20.2, 8.2, 6.5 Hz, 2H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.53 (s, 1H), 7.52 – 7.37 (m, 7H), 3.88 (d, *J* = 1.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 186.0, 183.7, 144.0, 143.9, 143.5, 142.5, 134.3, 134.2, 133.6, 133.2, 131.9, 128.2, 128.1, 128.1, 128.0, 126.8, 126.7, 126.6, 125.6, 122.3, 121.0, 120.7, 117.0, 108.7, 29.3. HRMS (ESI) Calcd for $C_{27}H_{18}NO_2^+[M+H]^+$: 388.1338, Found: 388.1339.

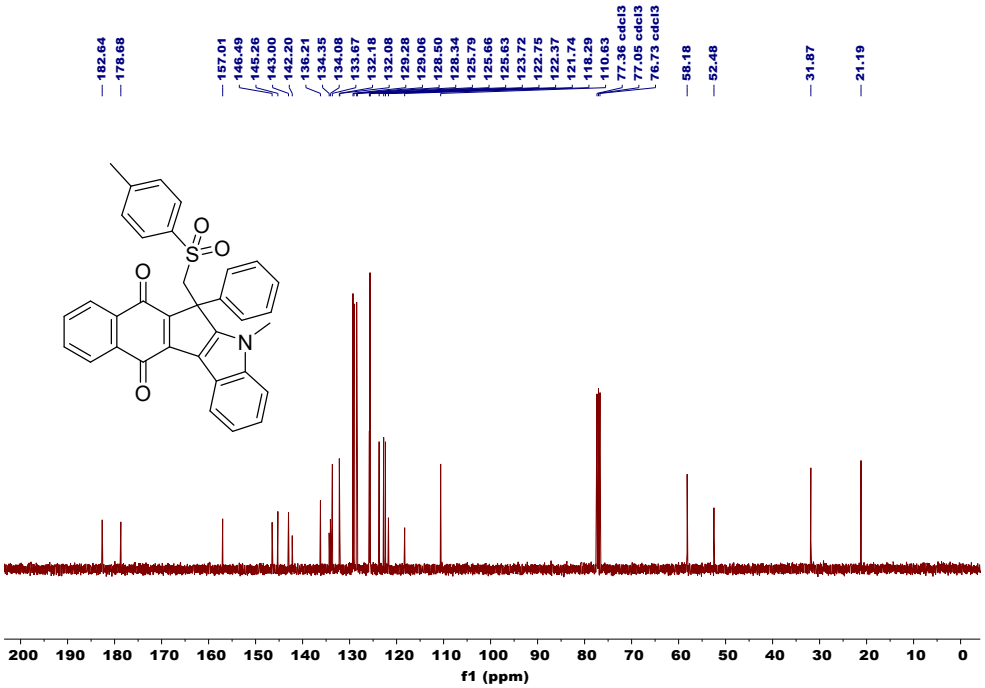
6. NMR Spectra of New Compounds

5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (5)

^{1}H NMR (400 MHz)

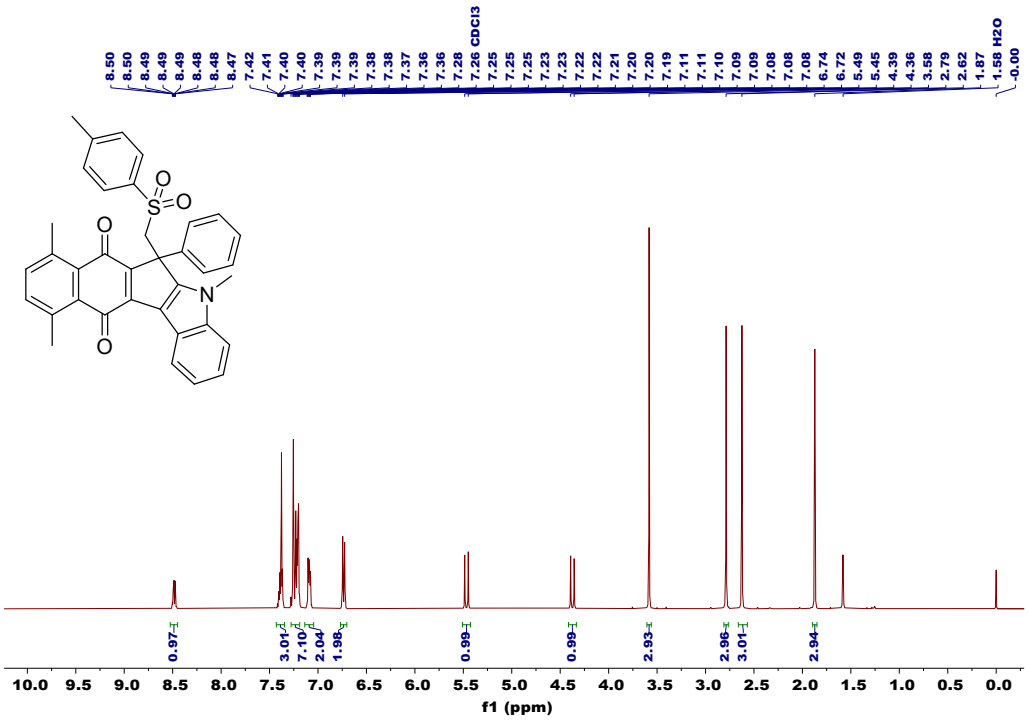


^{13}C {^{1}H} NMR (101 MHz)

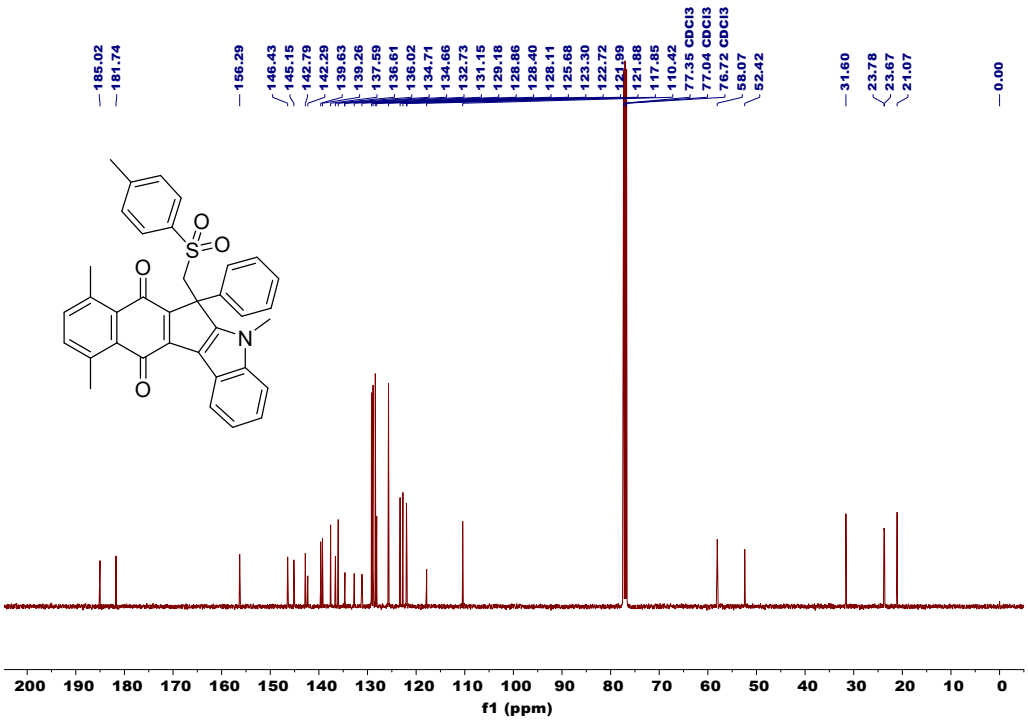


5,8,11-trimethyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (6)

^{1}H NMR (400 MHz)

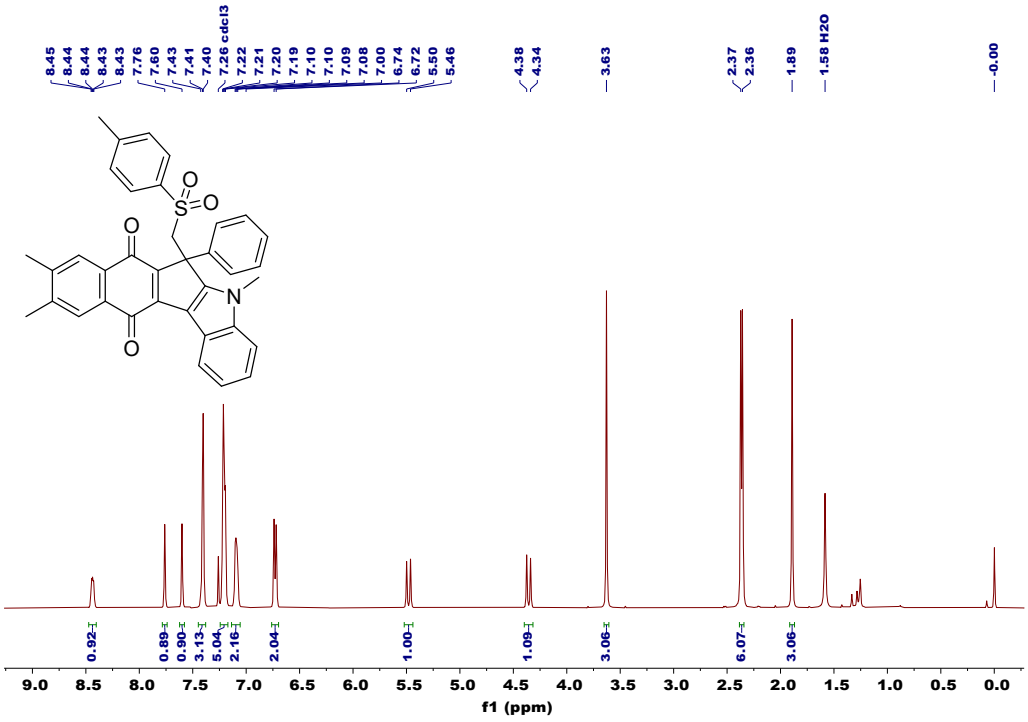


^{13}C {^{1}H} NMR (101 MHz)

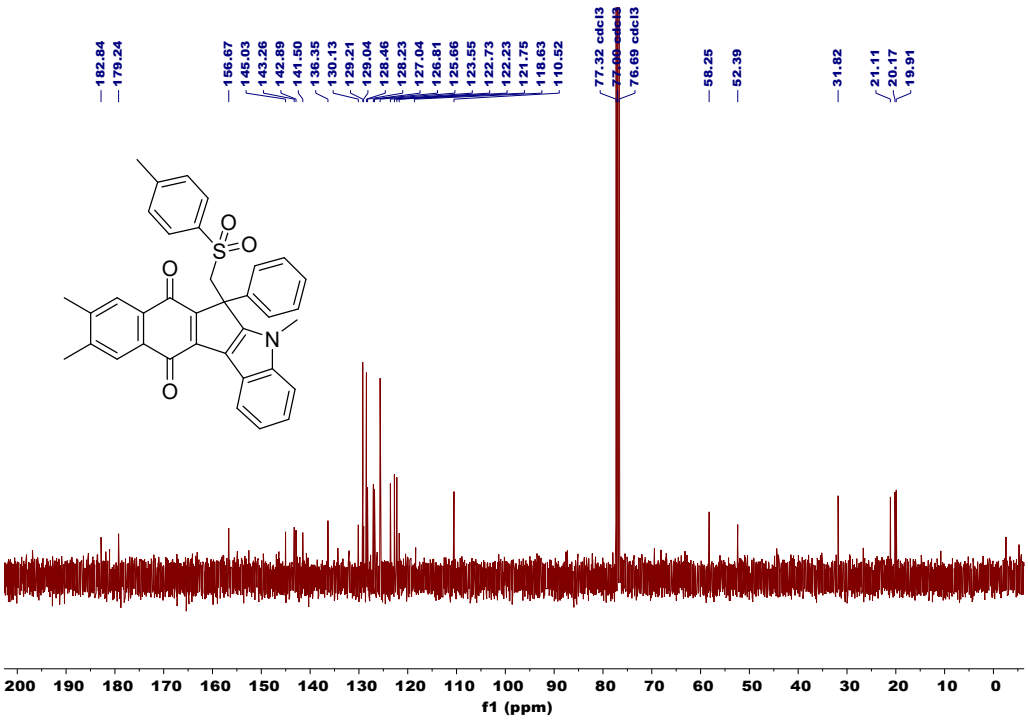


5,9,10-trimethyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (7)

^{1}H NMR (400 MHz)

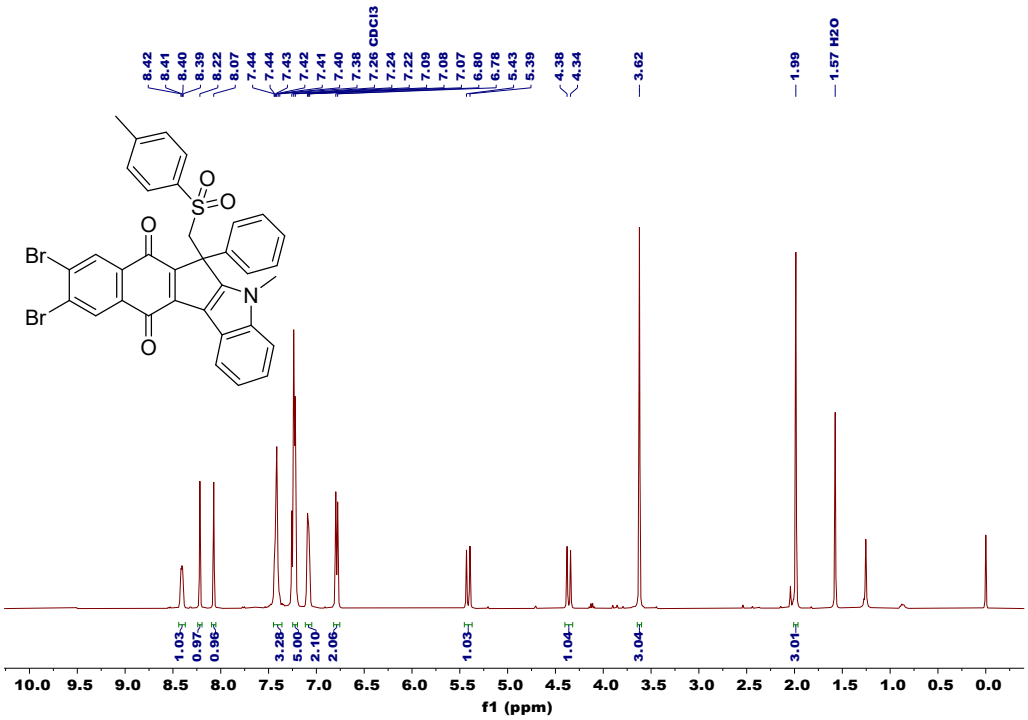


^{13}C {^{1}H} NMR (101 MHz)

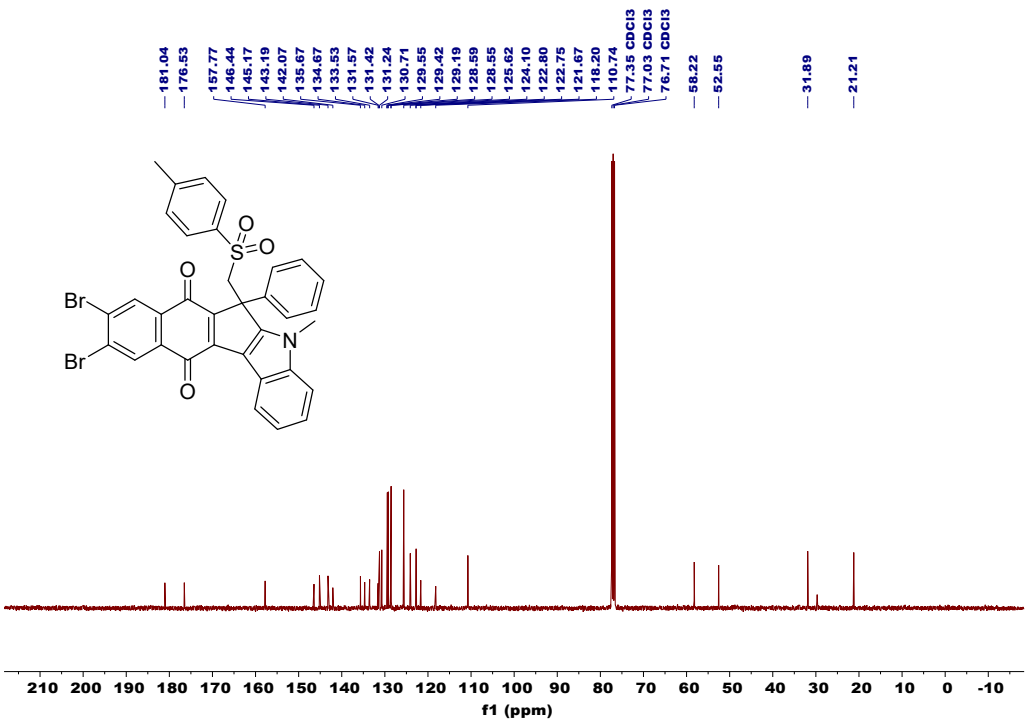


9,10-dibromo-5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (8)

^{1}H NMR (400 MHz)

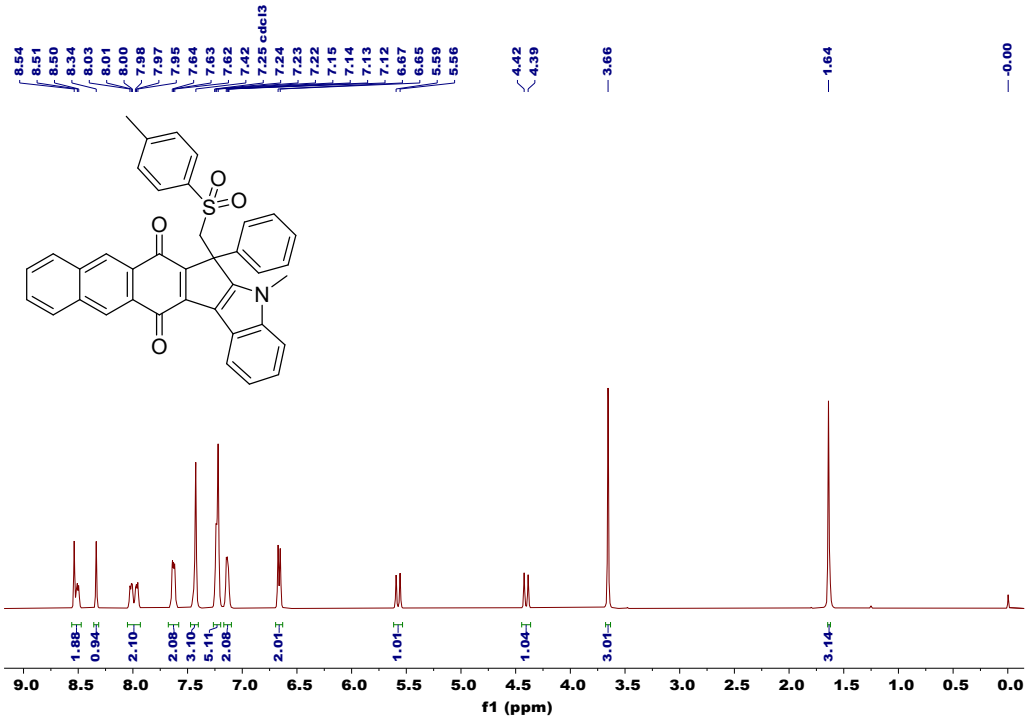


^{13}C {^{1}H} NMR (101 MHz)

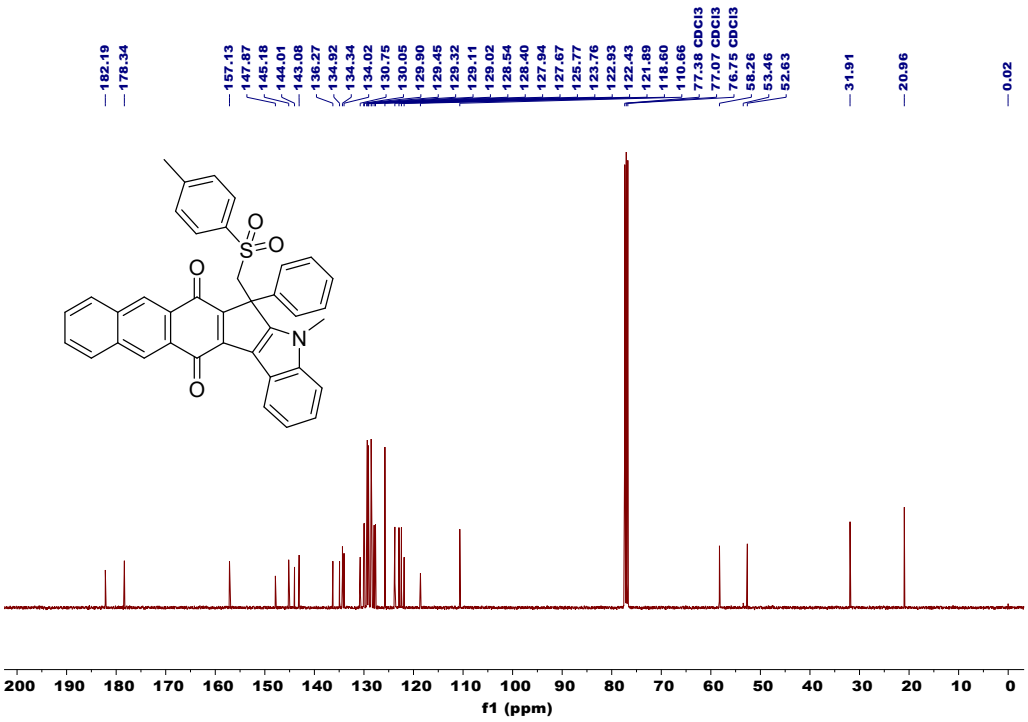


5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydronaphtho[2',3':5,6]indeno[2,1-*b*]indole-7,14-dione (9)

^{1}H NMR (400 MHz)

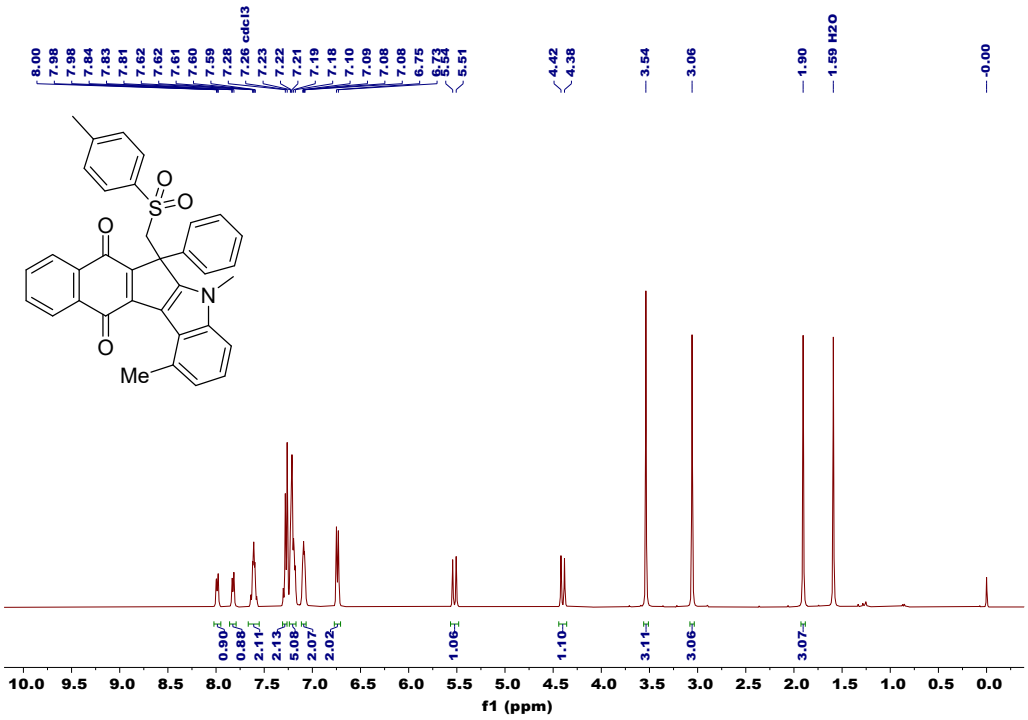


^{13}C {^{1}H} NMR (101 MHz)

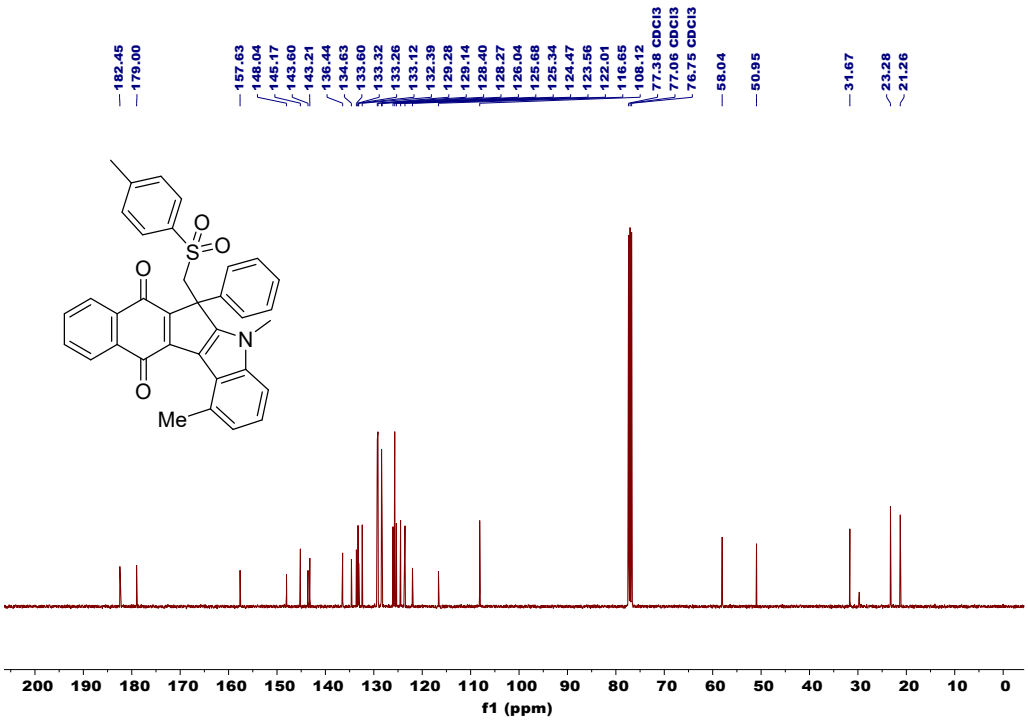


1,5-dimethyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (10)

^{1}H NMR (400 MHz)

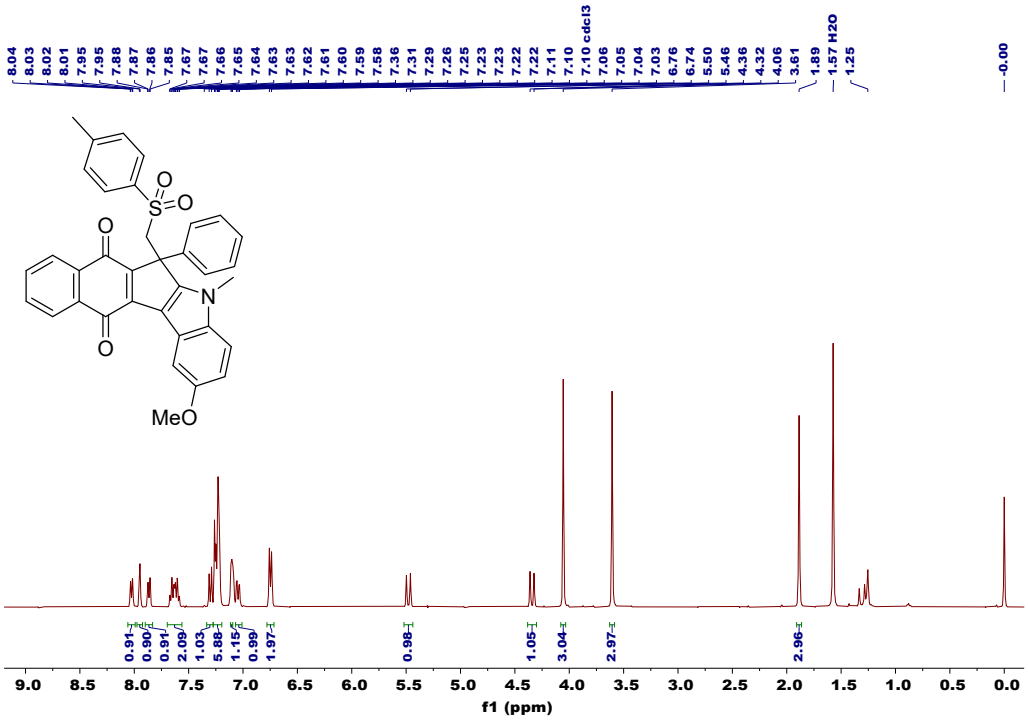


^{13}C {^{1}H} NMR (101 MHz)

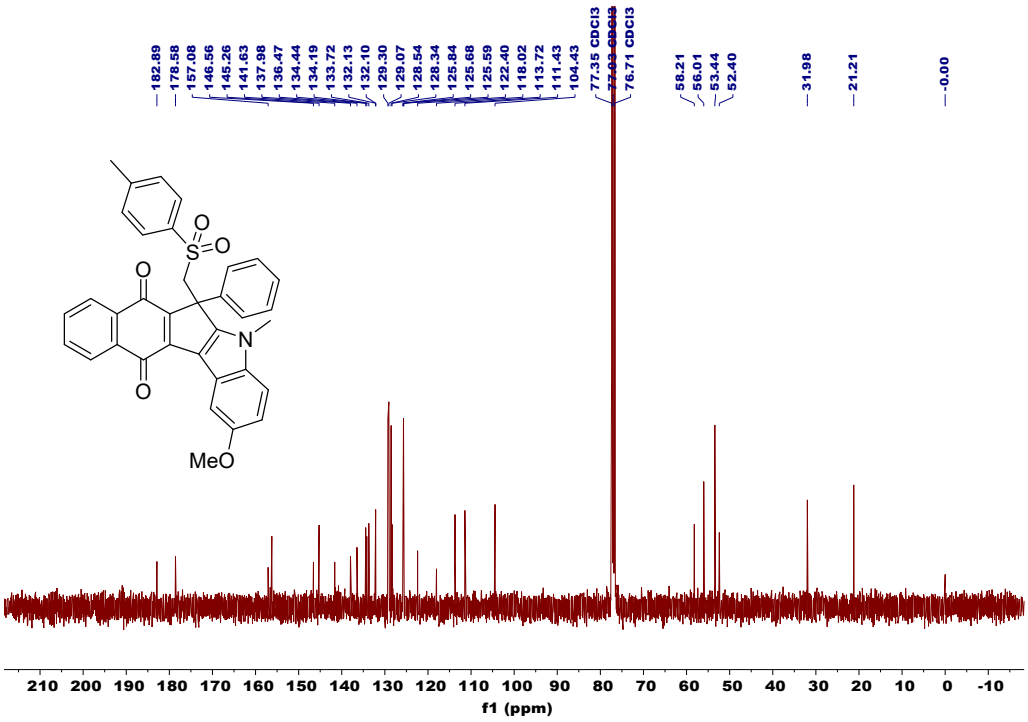


2-methoxy-5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (11)

^{1}H NMR (400 MHz)

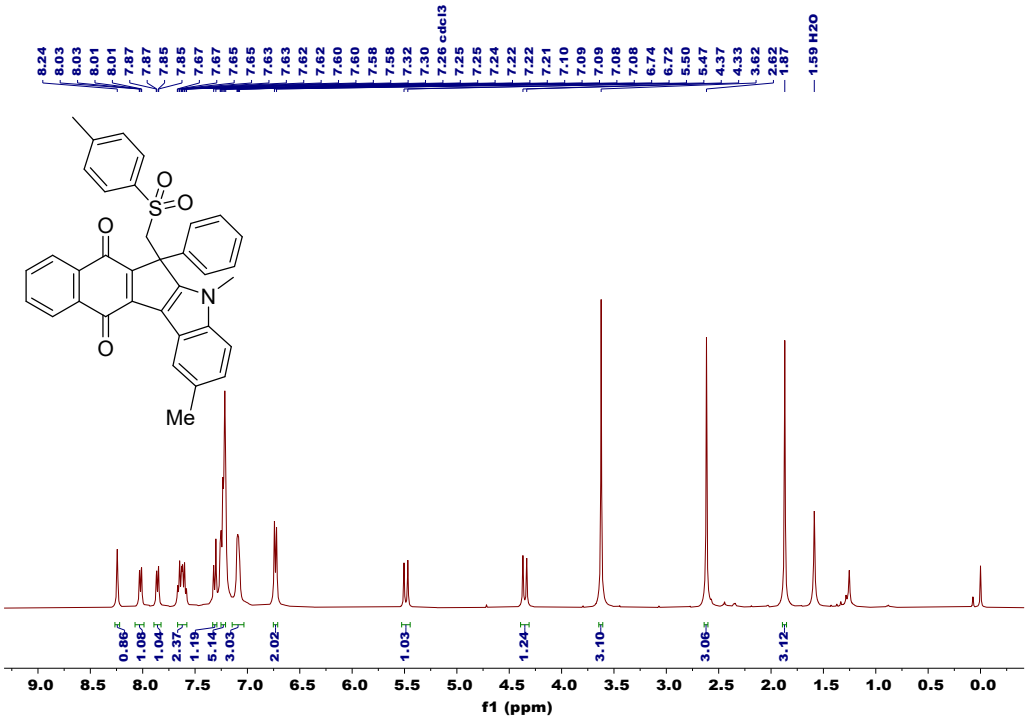


^{13}C {^{1}H} NMR (101 MHz)

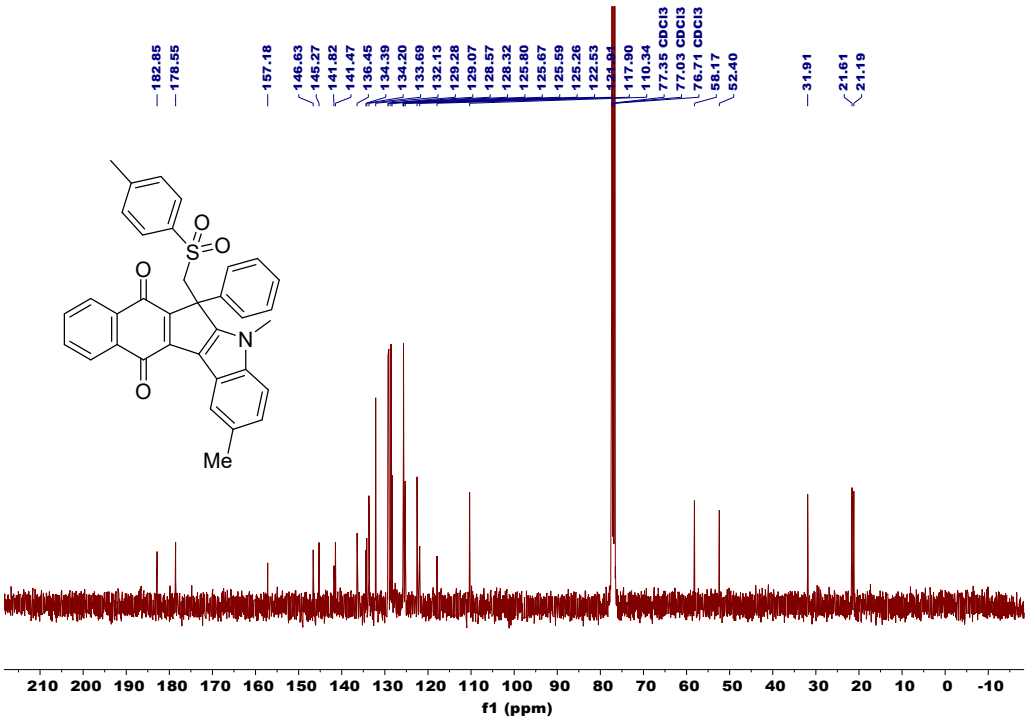


2,5-dimethyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (12)

^{1}H NMR (400 MHz)

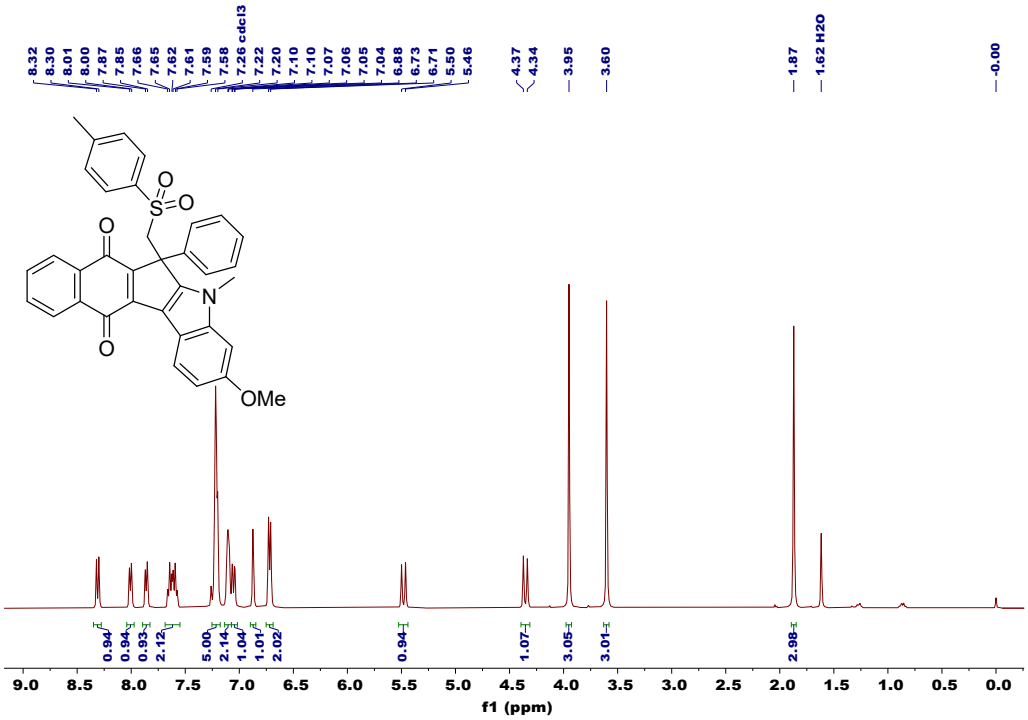


^{13}C {^{1}H} NMR (101 MHz)

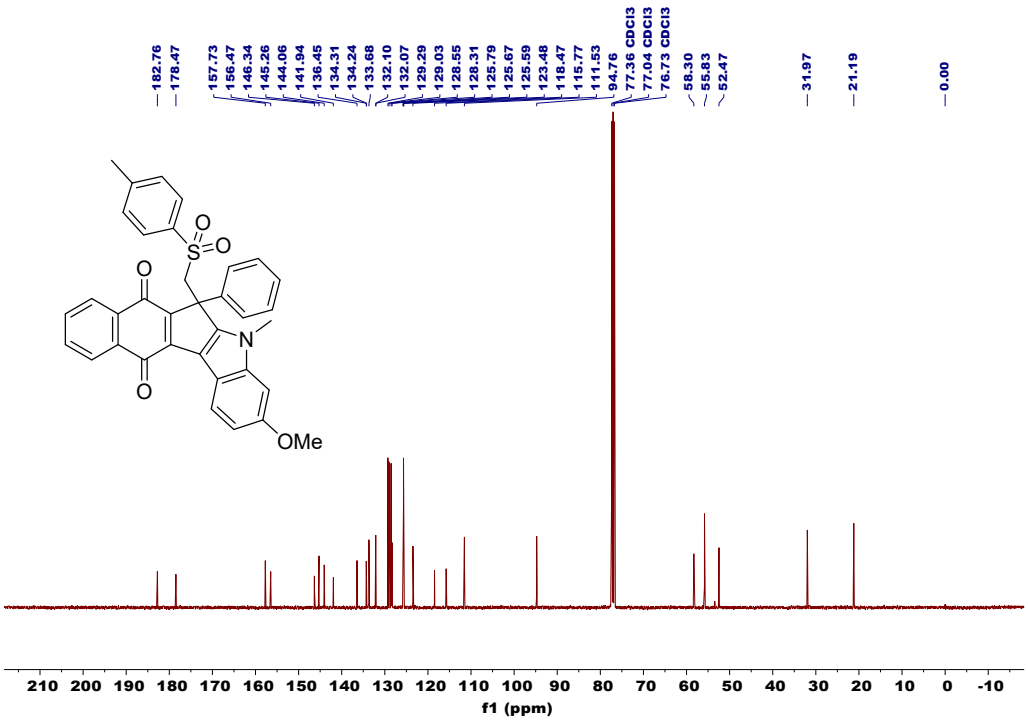


3-methoxy-5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (13)

^{1}H NMR (400 MHz)

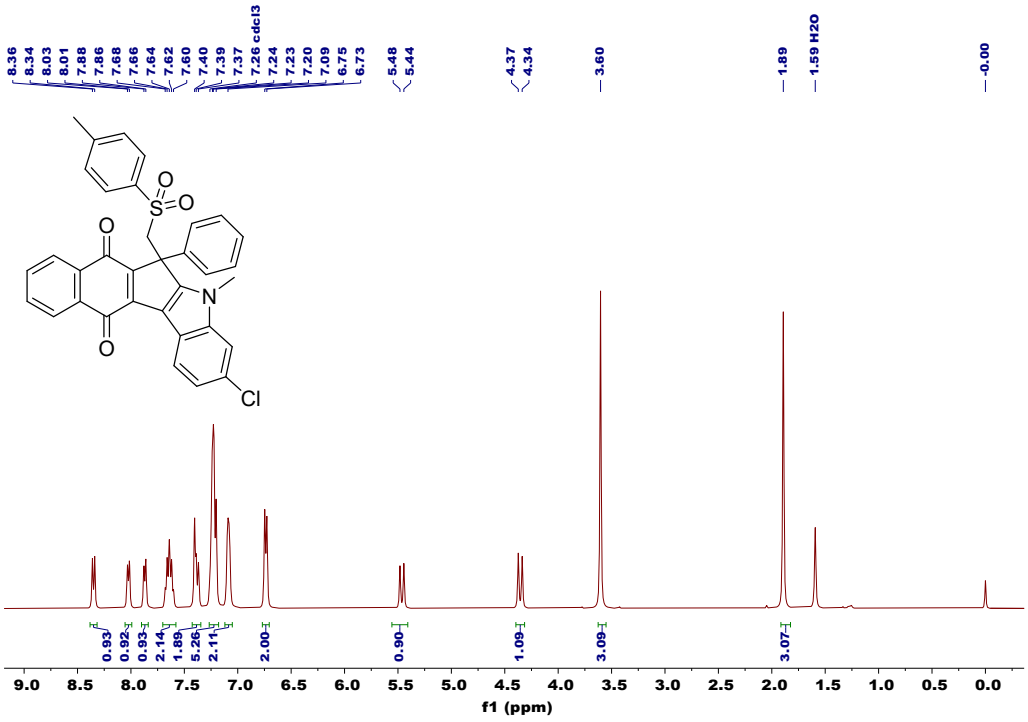


^{13}C {^{1}H} NMR (101 MHz)

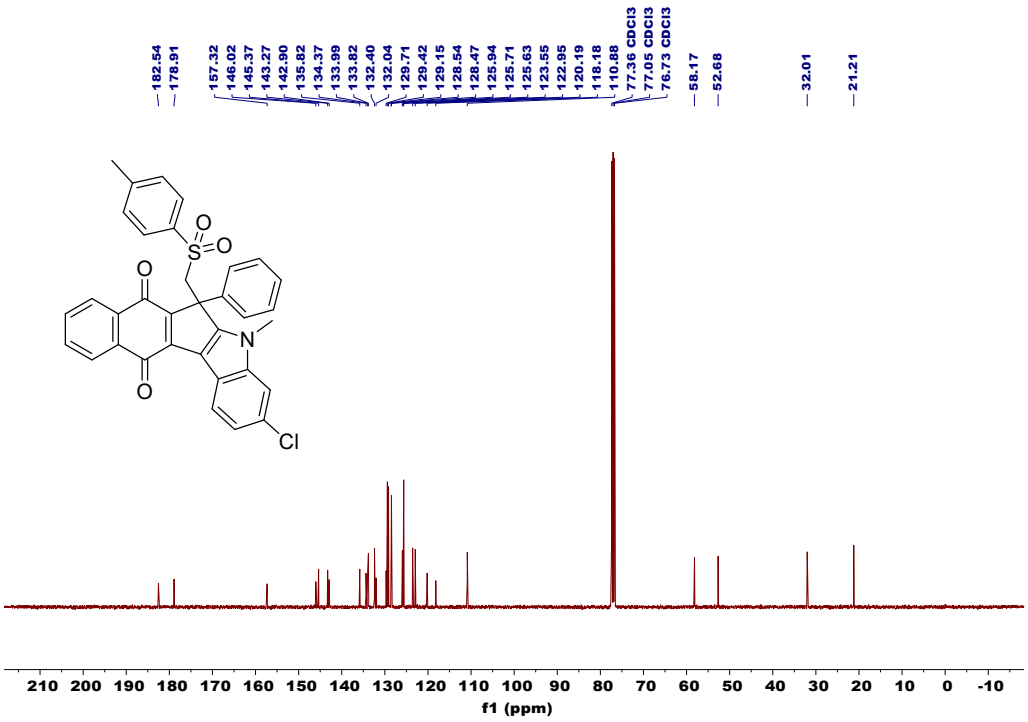


3-chloro-5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (14)

^{1}H NMR (400 MHz)

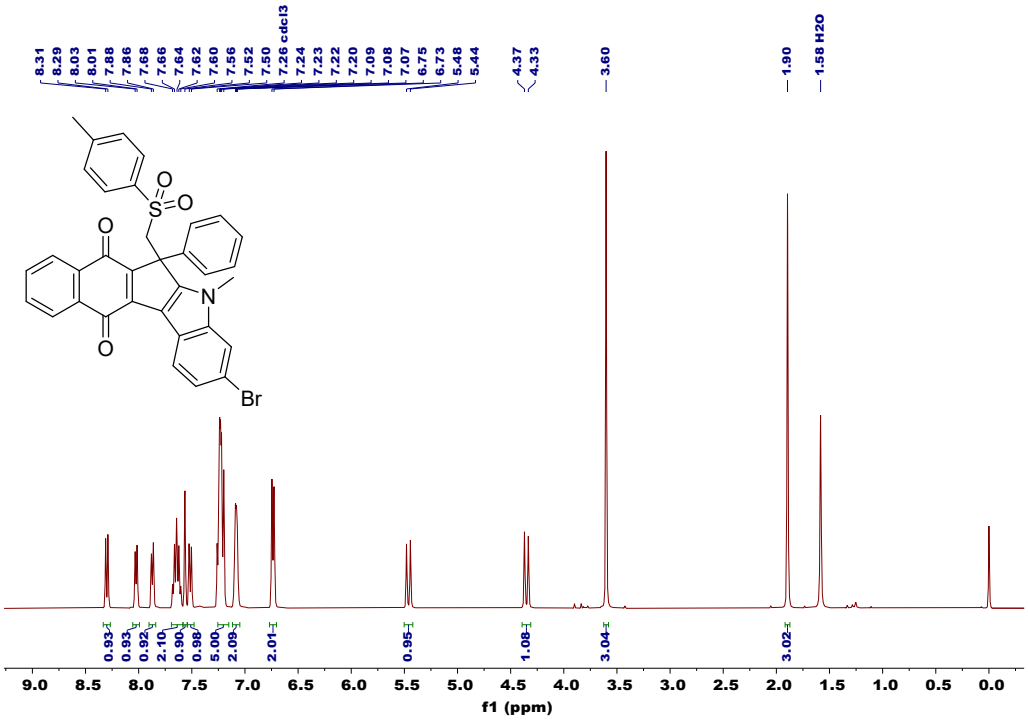


^{13}C {^{1}H} NMR (101 MHz)

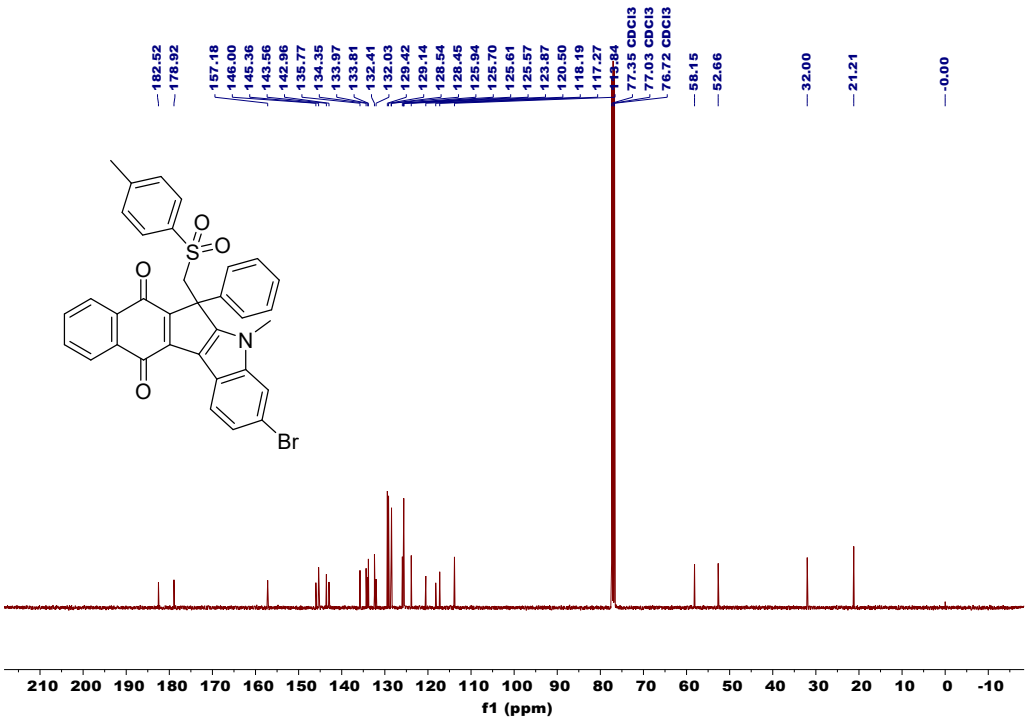


3-bromo-5-methyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (15)

^{1}H NMR (400 MHz)

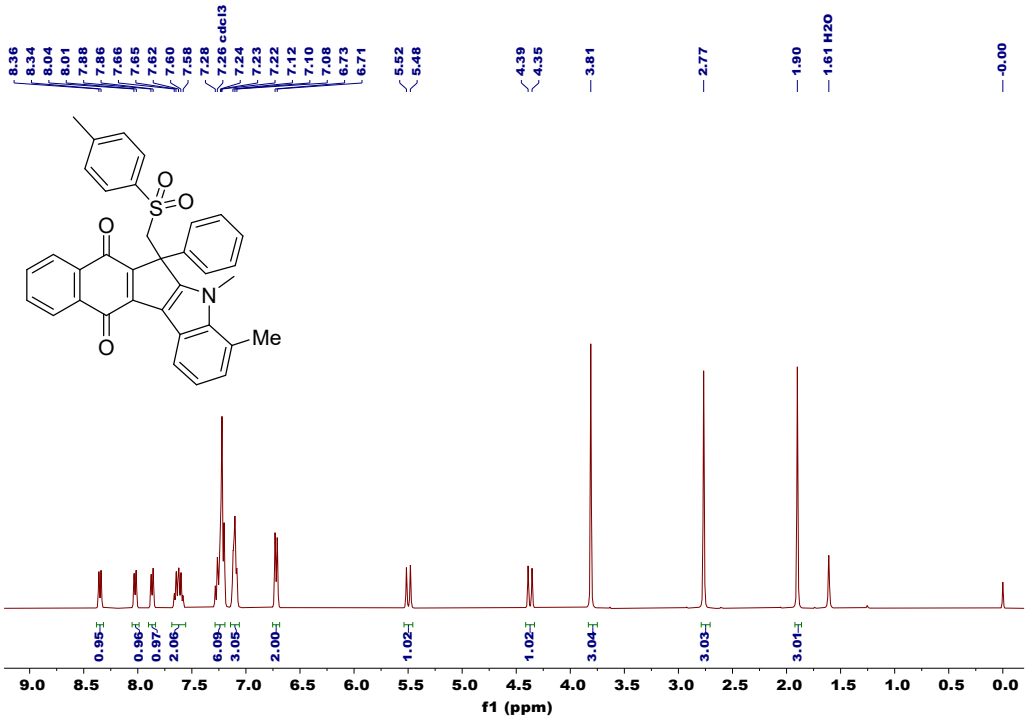


^{13}C {^{1}H} NMR (101 MHz)

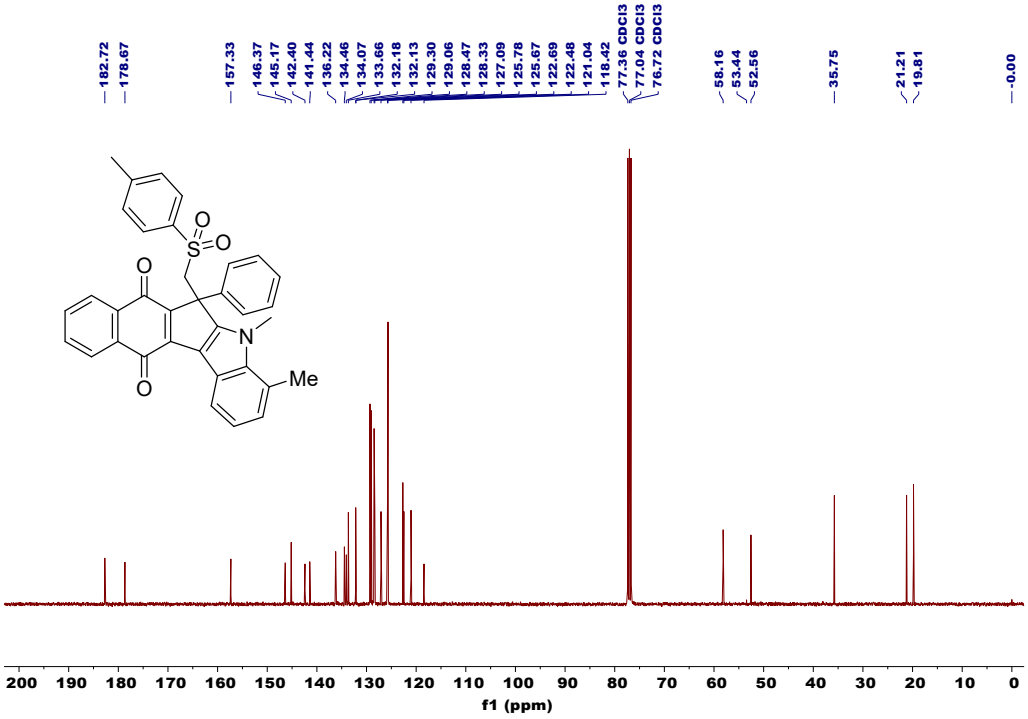


4,5-dimethyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (16)

^{1}H NMR (400 MHz)

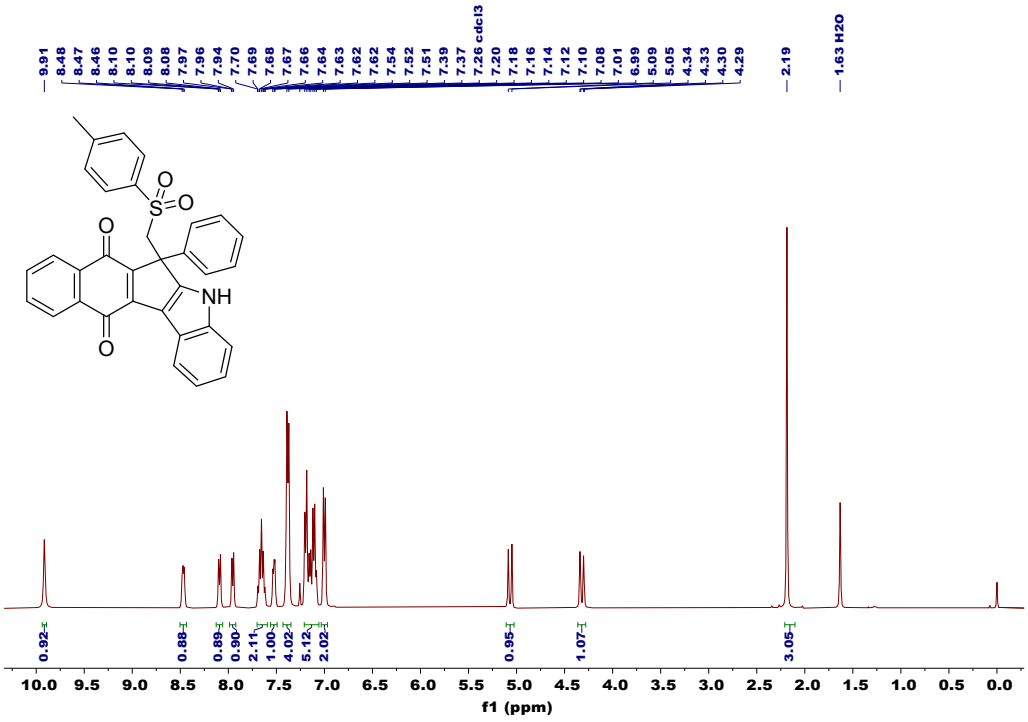


^{13}C {^{1}H} NMR (101 MHz)

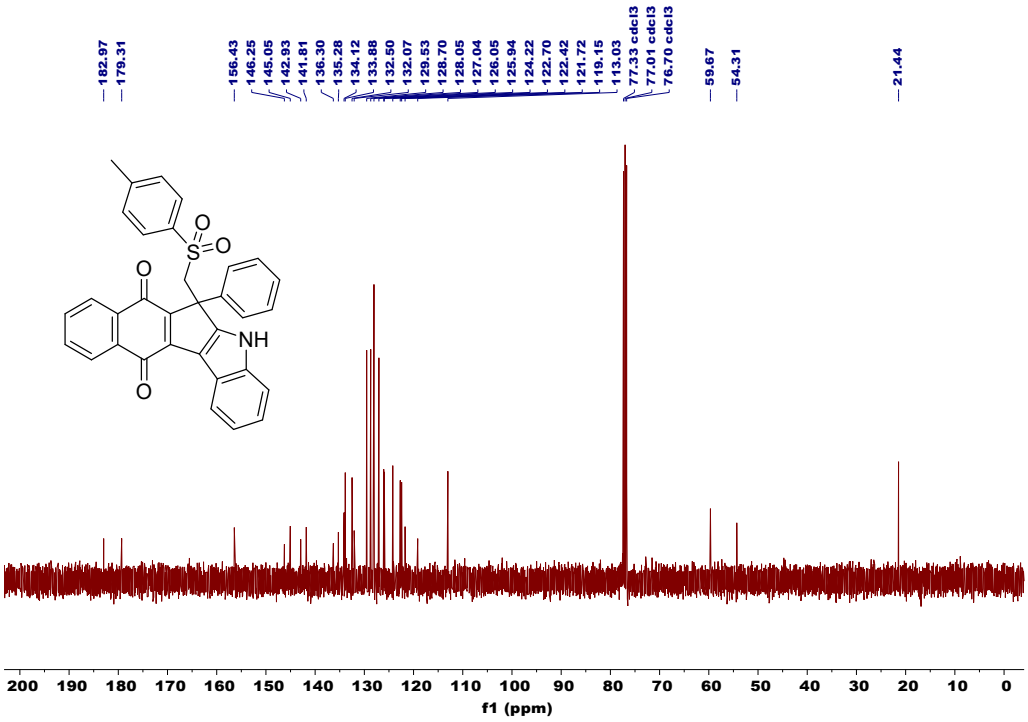


6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (17)

^{1}H NMR (400 MHz)

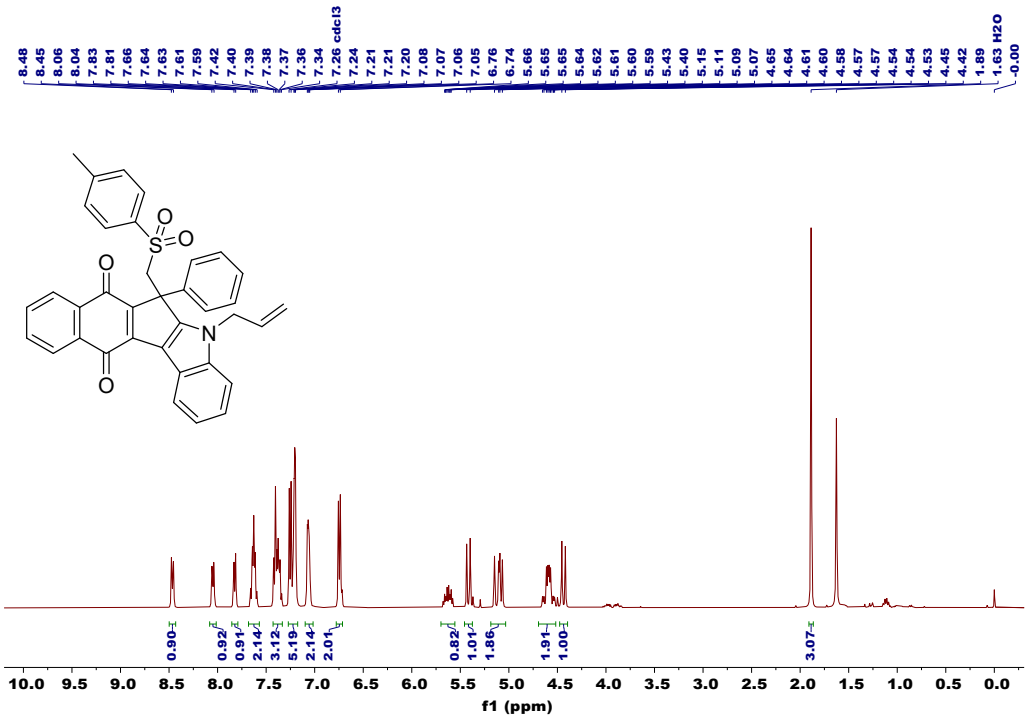


^{13}C {^{1}H} NMR (101 MHz)

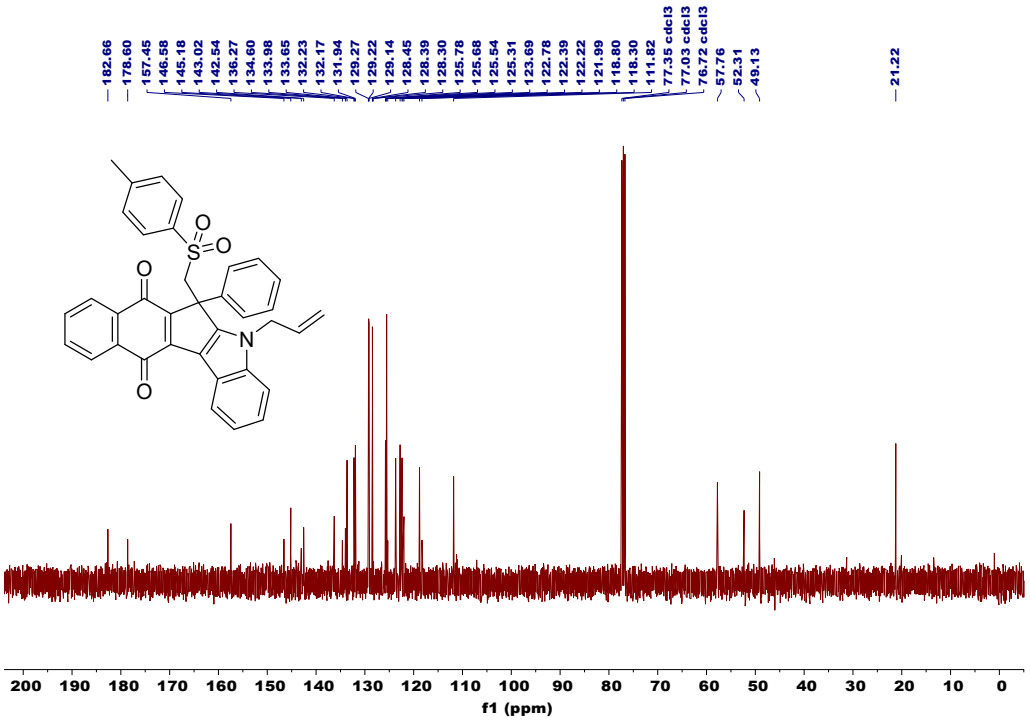


5-allyl-6-phenyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (19)

^{1}H NMR (400 MHz)

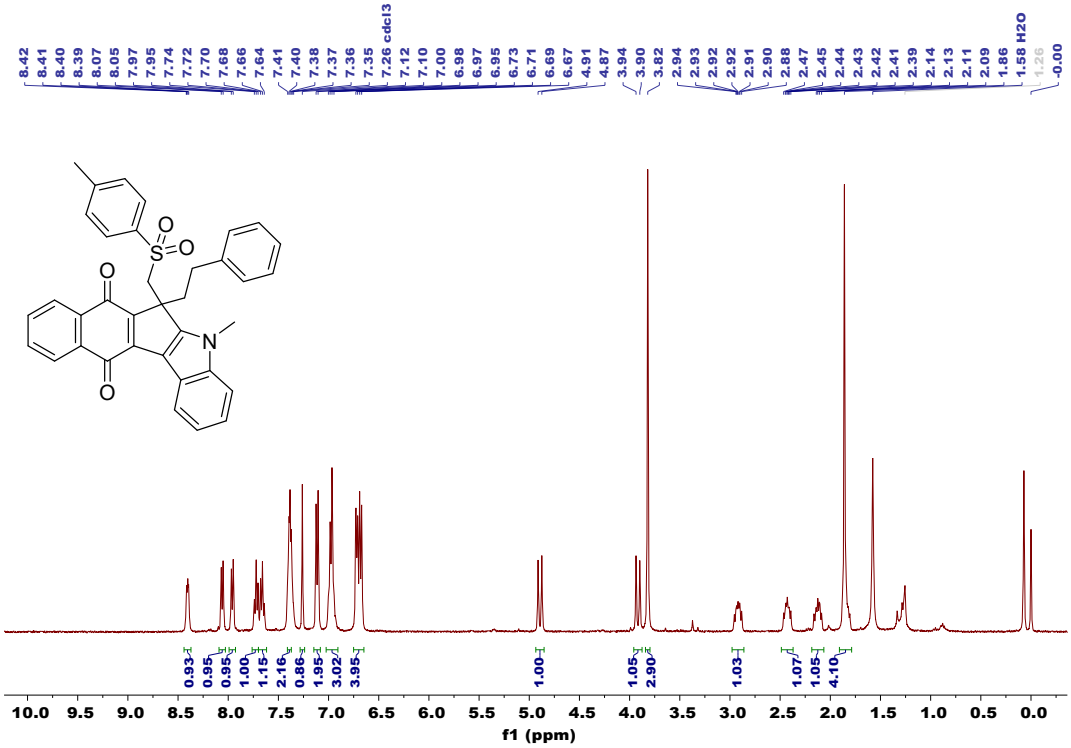


^{13}C {^{1}H} NMR (101 MHz)

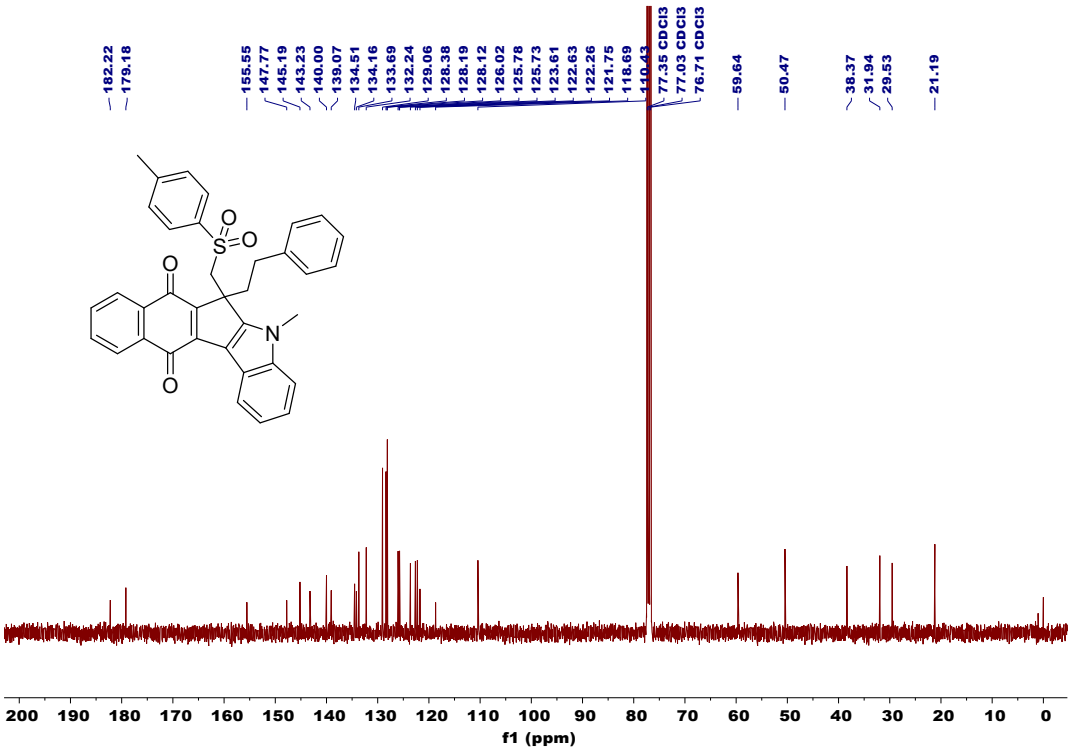


5-methyl-6-phenethyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (20)

^{1}H NMR (400 MHz)

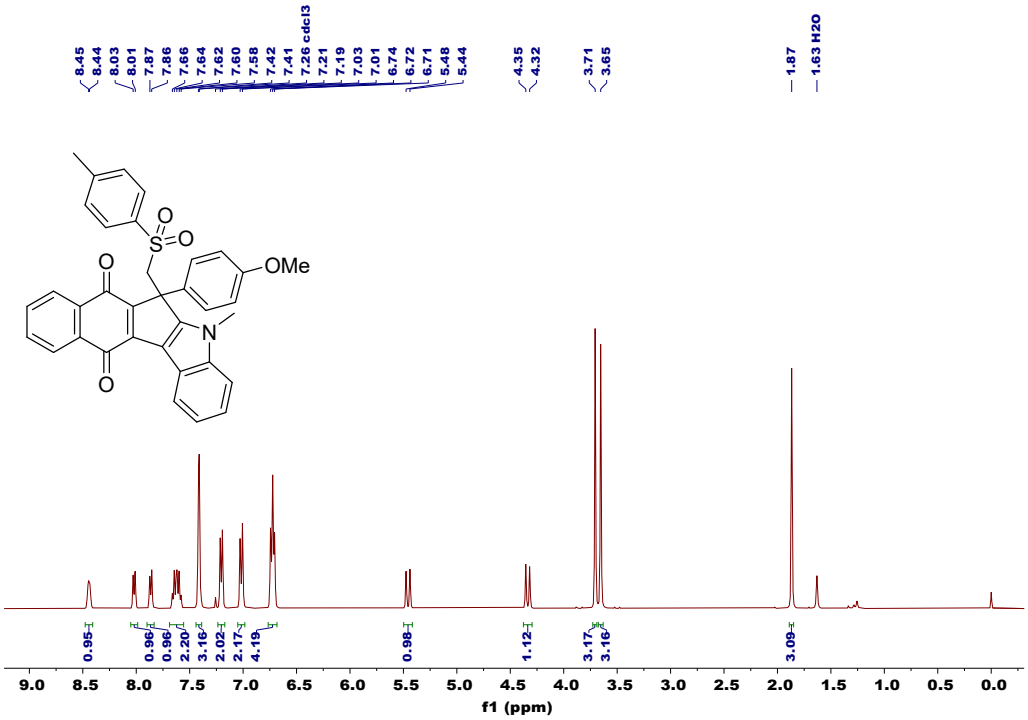


^{13}C {^{1}H} NMR (101 MHz)

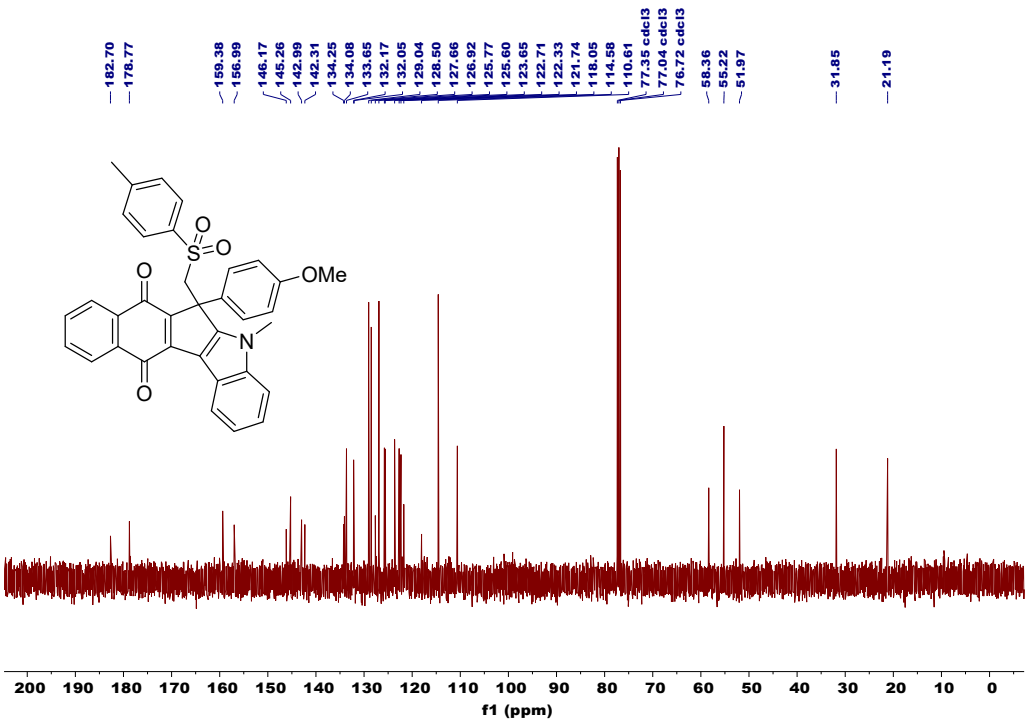


6-(4-methoxyphenyl)-5-methyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (21)

^{1}H NMR (400 MHz)

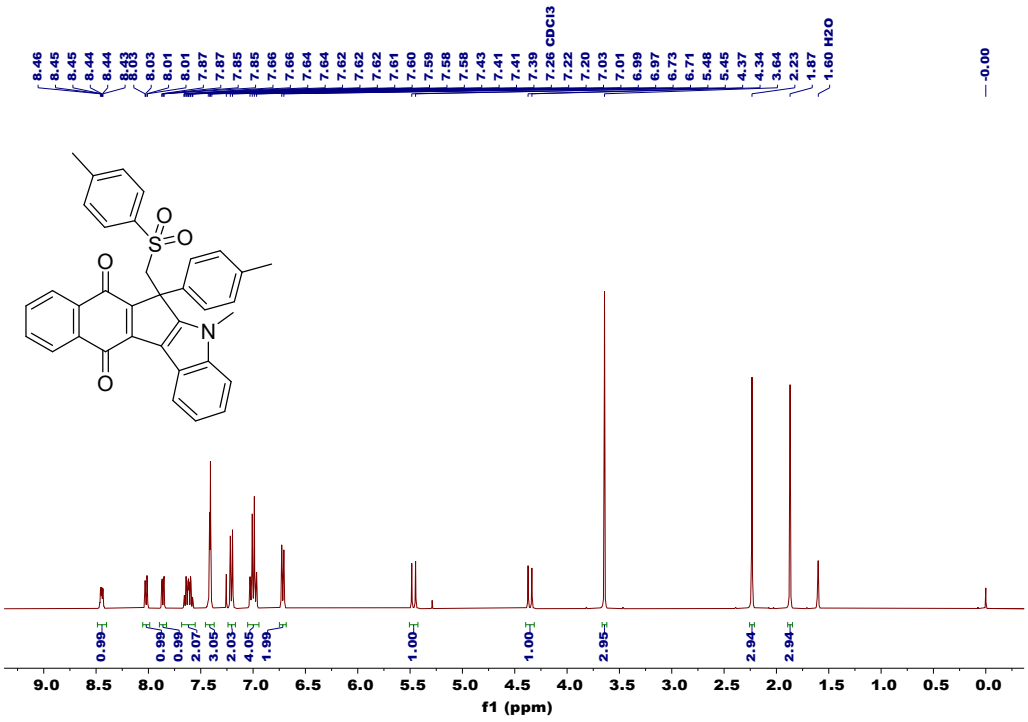


^{13}C {^{1}H} NMR (101 MHz)

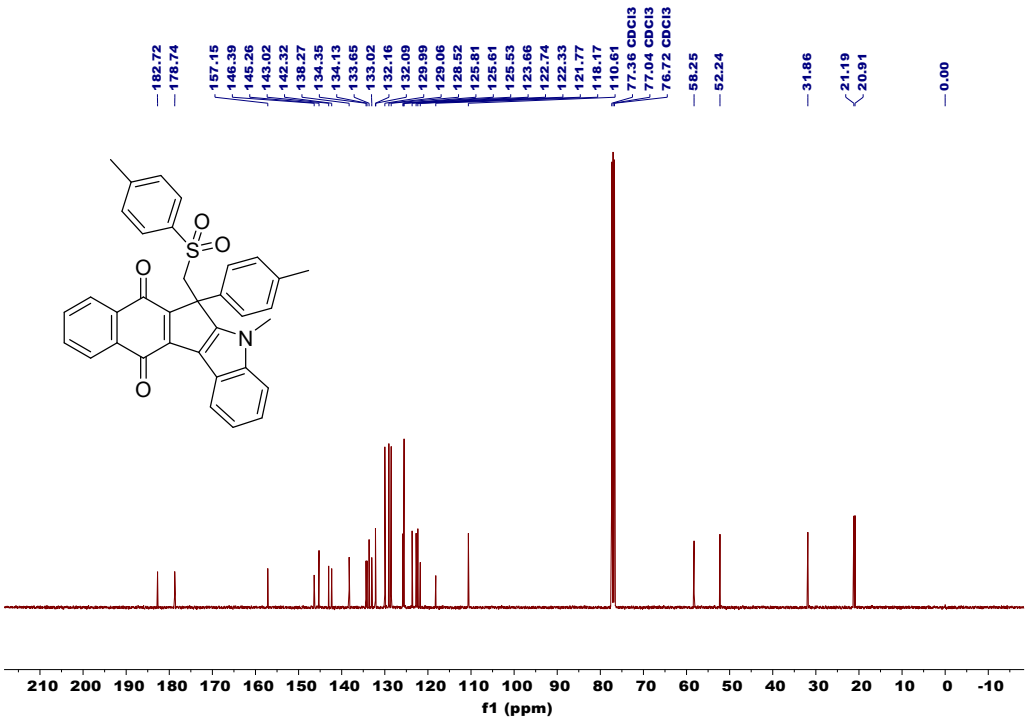


5-methyl-6-(p-tolyl)-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (22)

^{1}H NMR (400 MHz)

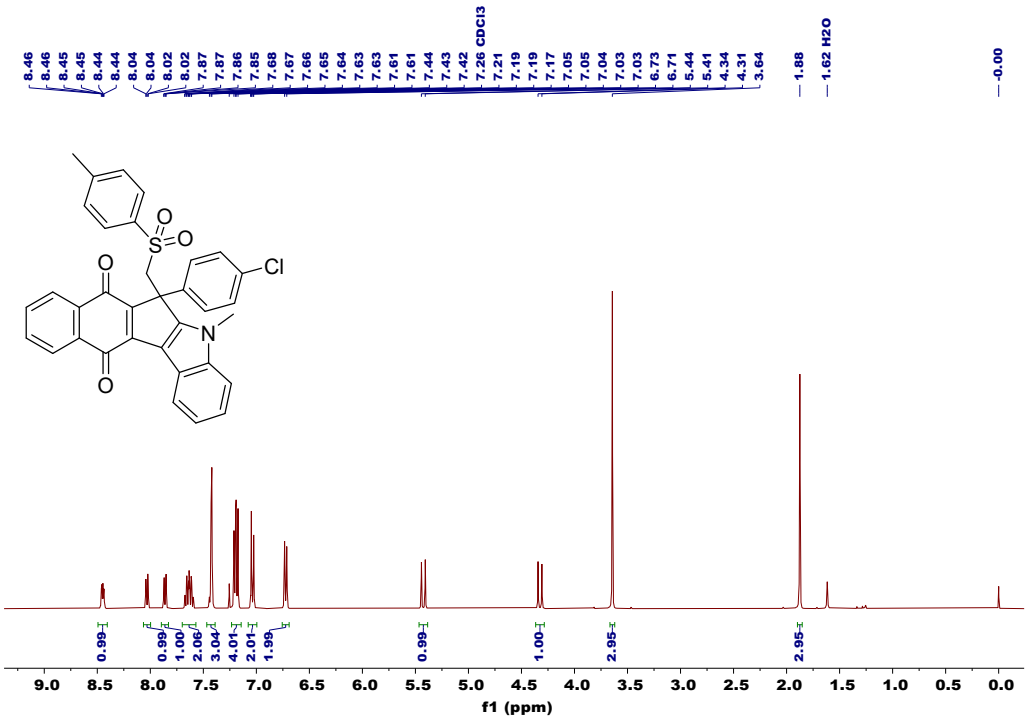


^{13}C {^{1}H} NMR (101 MHz)

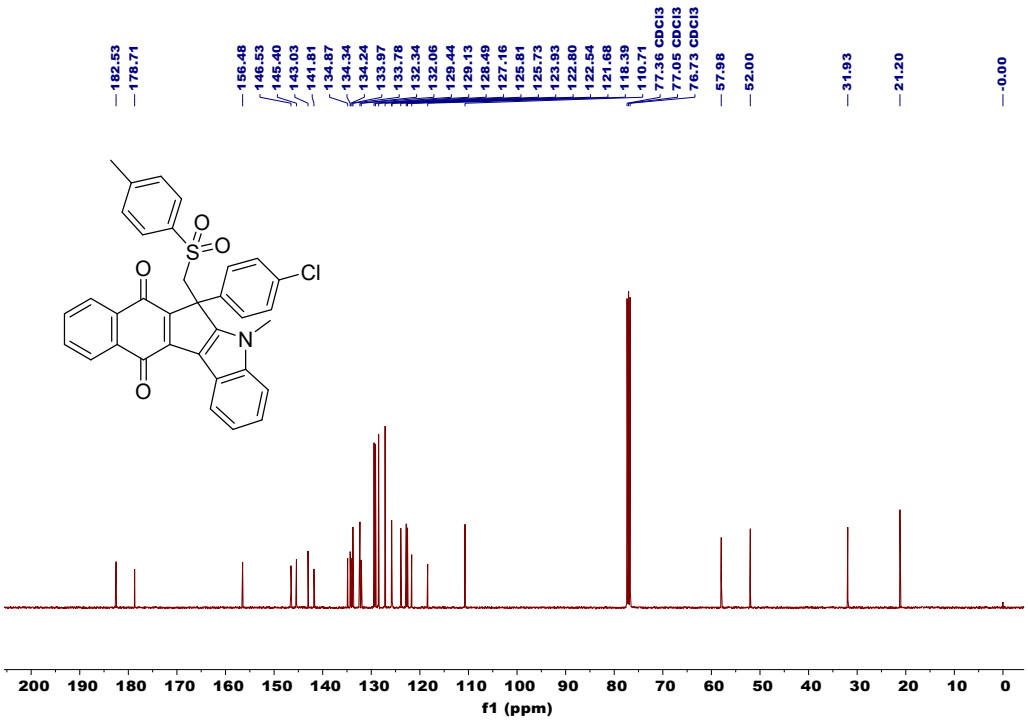


6-(4-chlorophenyl)-5-methyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (23)

^{1}H NMR (400 MHz)

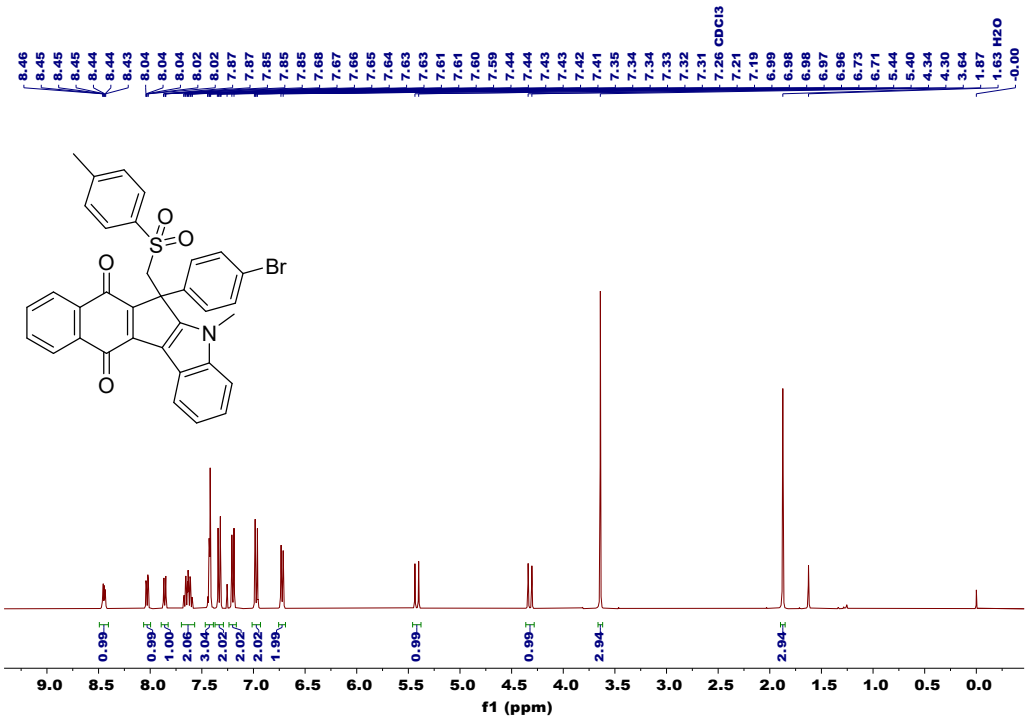


^{13}C {^{1}H} NMR (101 MHz)

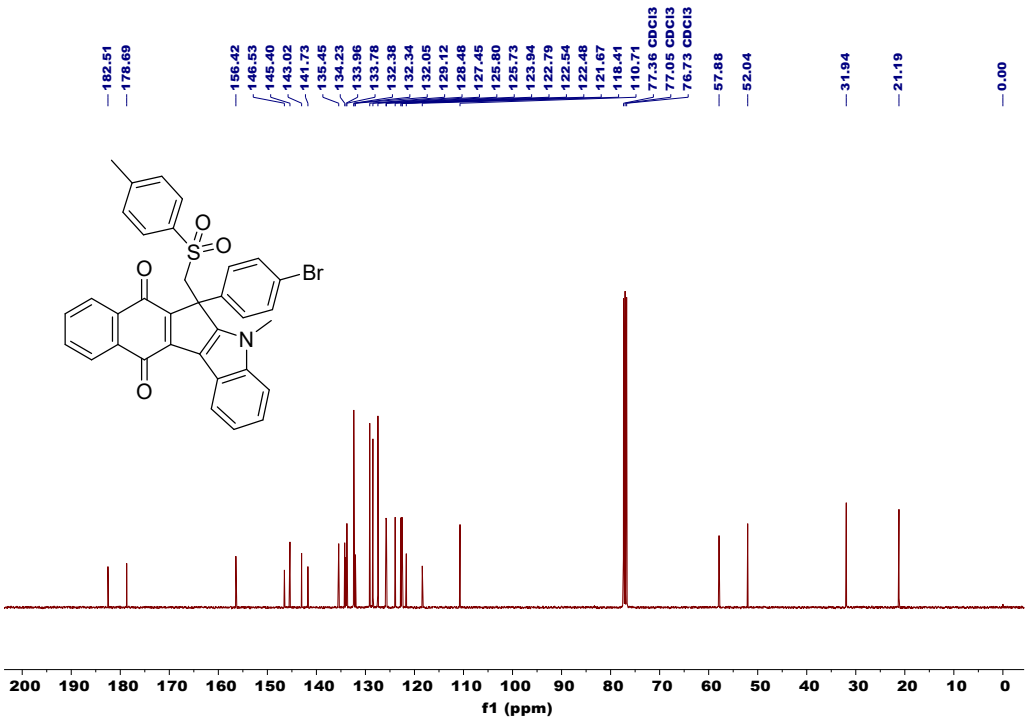


6-(4-bromophenyl)-5-methyl-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (24)

^{1}H NMR (400 MHz)

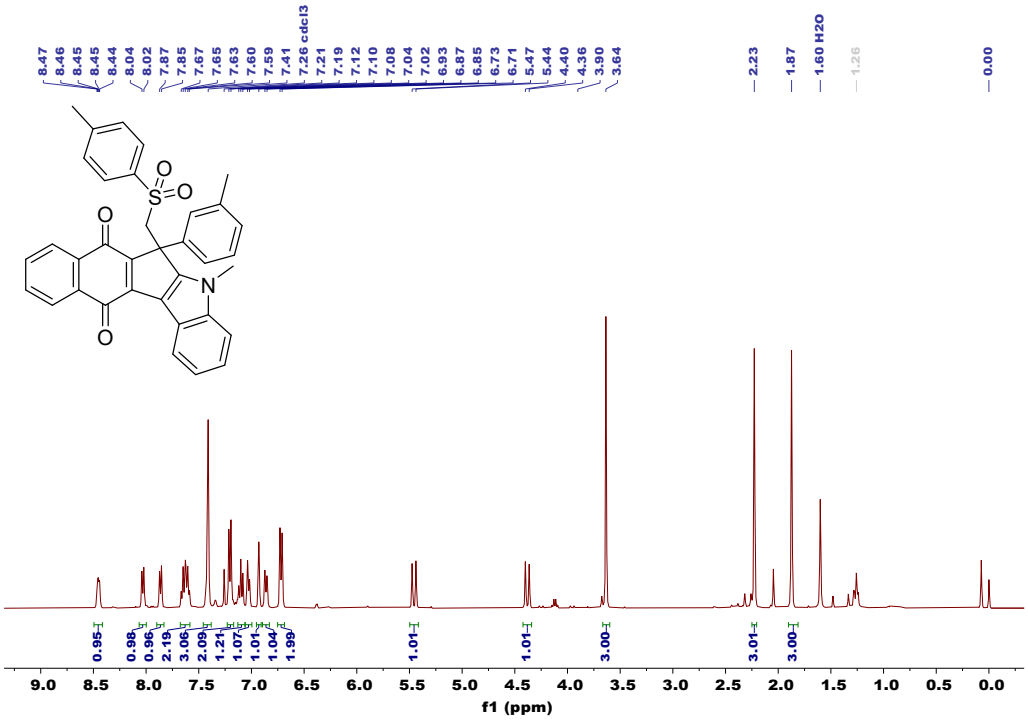


^{13}C {^{1}H} NMR (101 MHz)

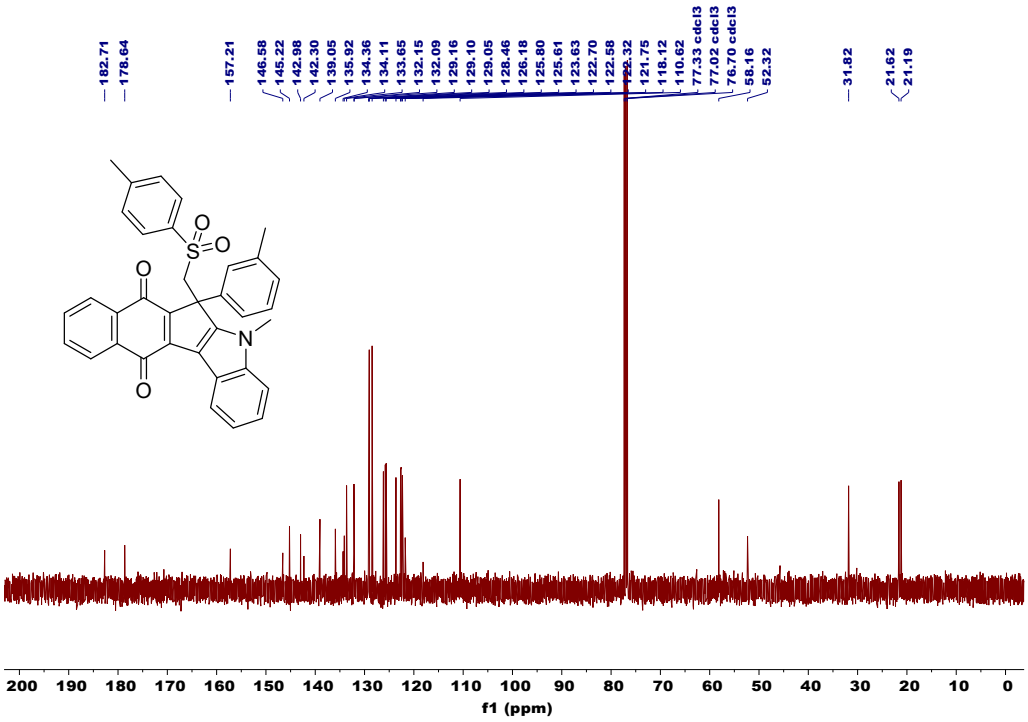


5-methyl-6-(m-tolyl)-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (25)

^{1}H NMR (400 MHz)

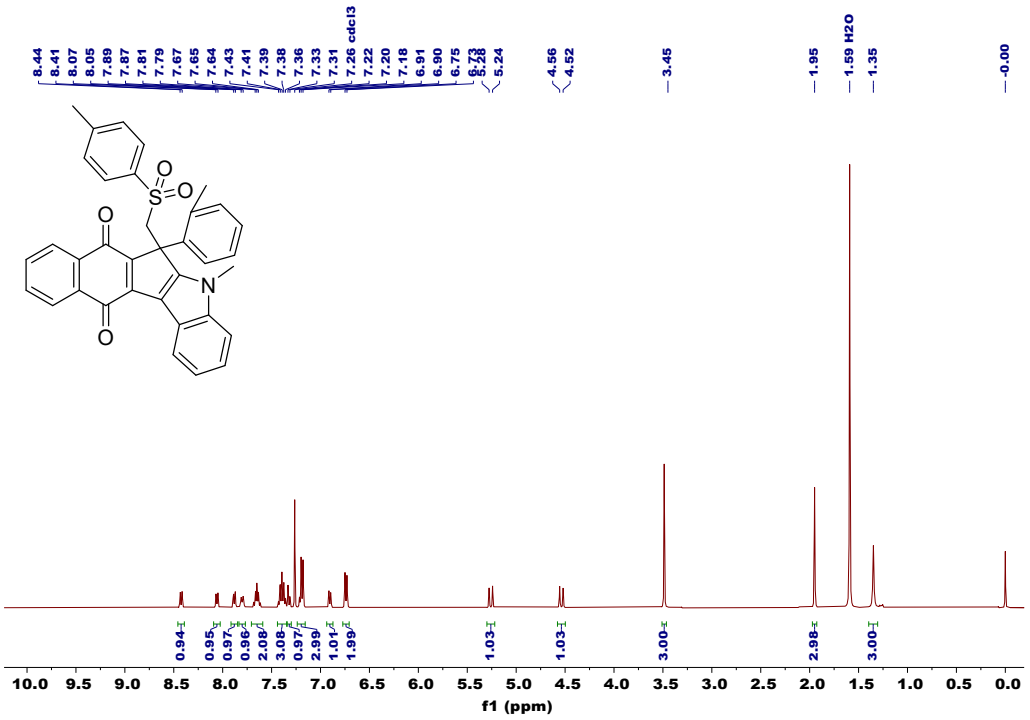


^{13}C {^{1}H} NMR (101 MHz)

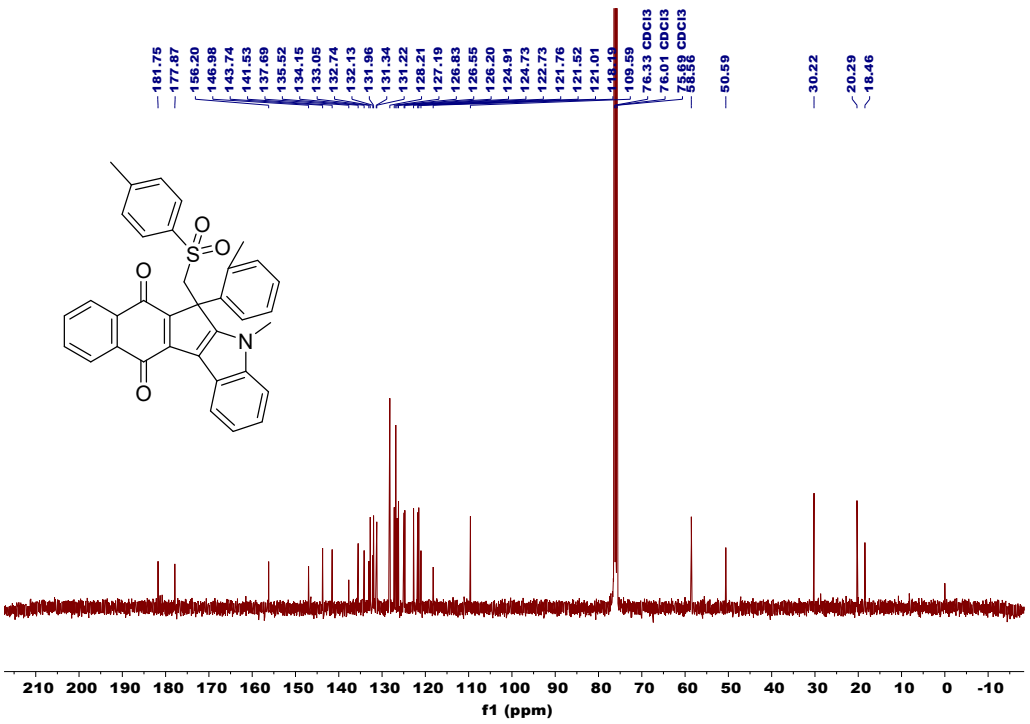


5-methyl-6-(o-tolyl)-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (26)

^{1}H NMR (400 MHz)

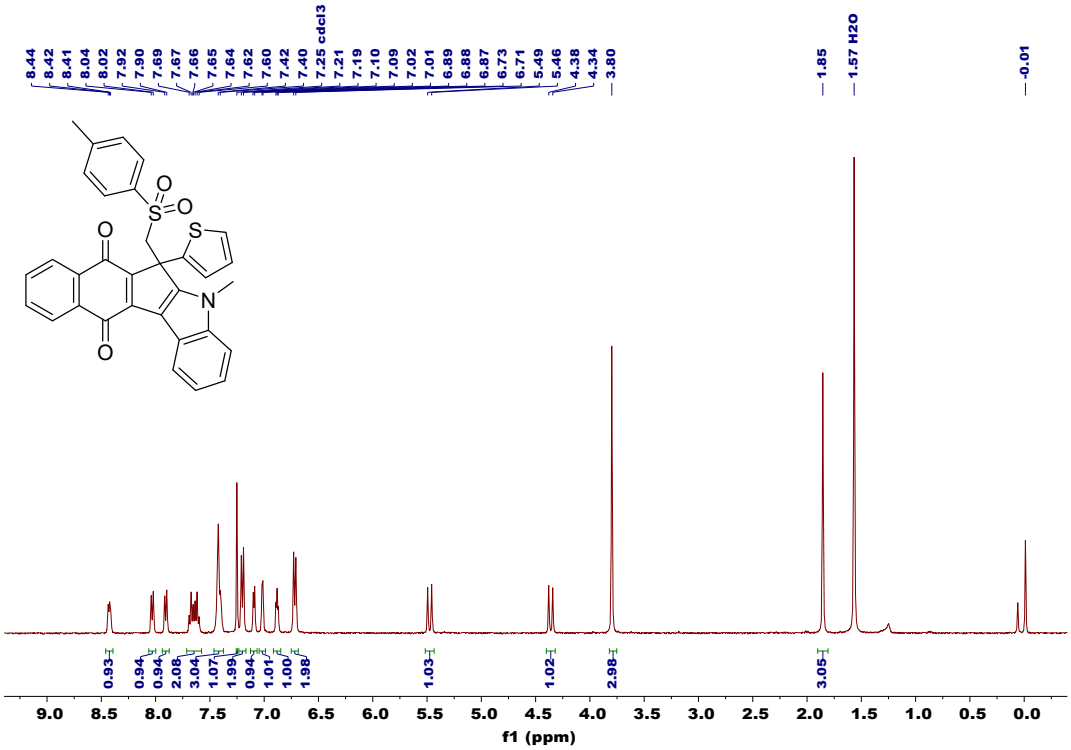


^{13}C {^{1}H} NMR (101 MHz)

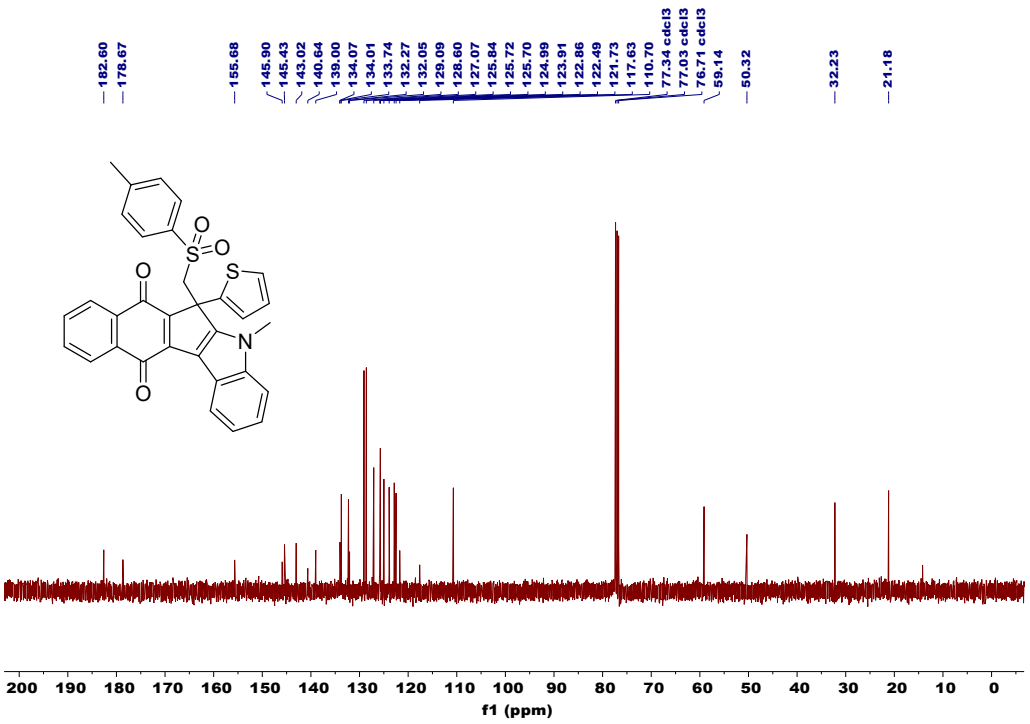


5-methyl-6-(thiophen-2-yl)-6-(tosylmethyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (27)

^{1}H NMR (400 MHz)

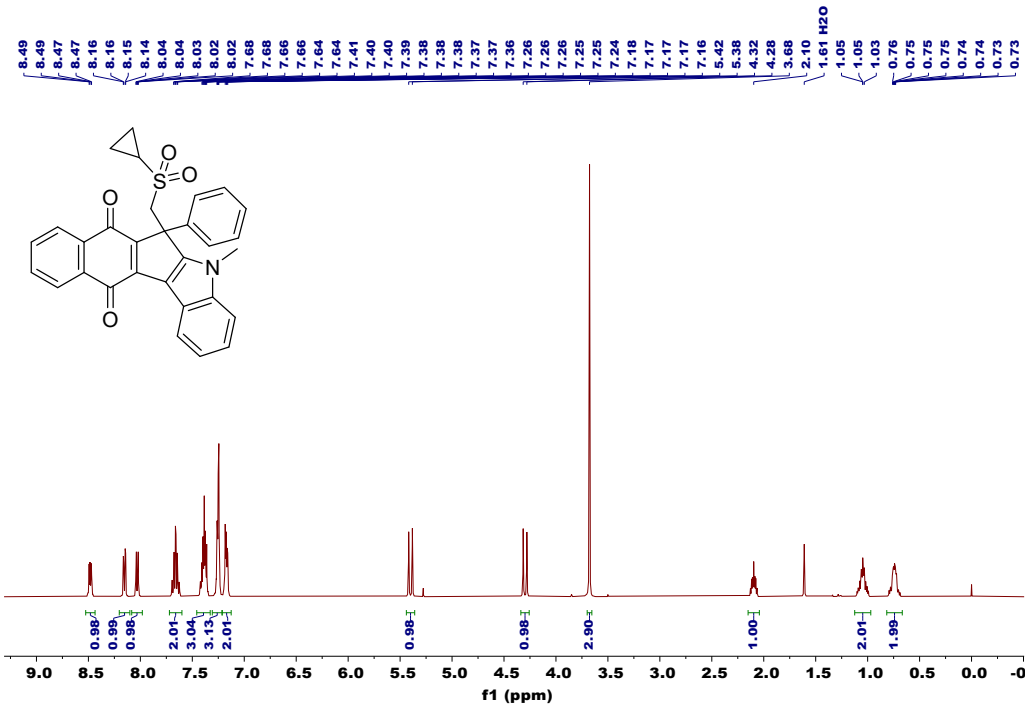


^{13}C {^{1}H} NMR (101 MHz)

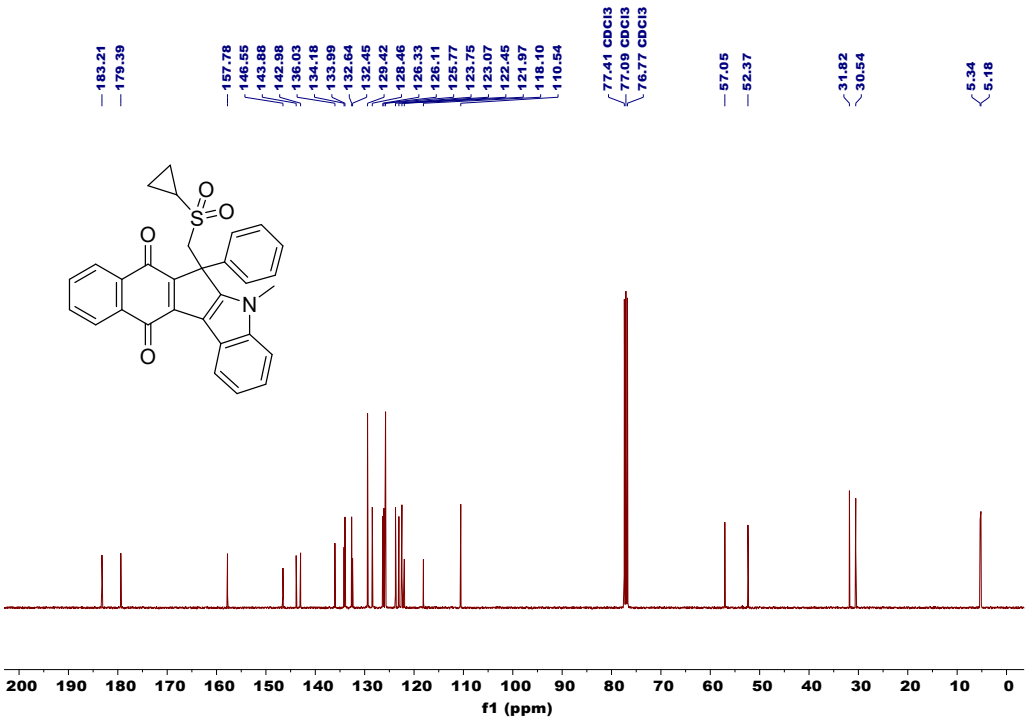


6-((cyclopropylsulfonyl)methyl)-5-methyl-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (28)

^{1}H NMR (400 MHz)

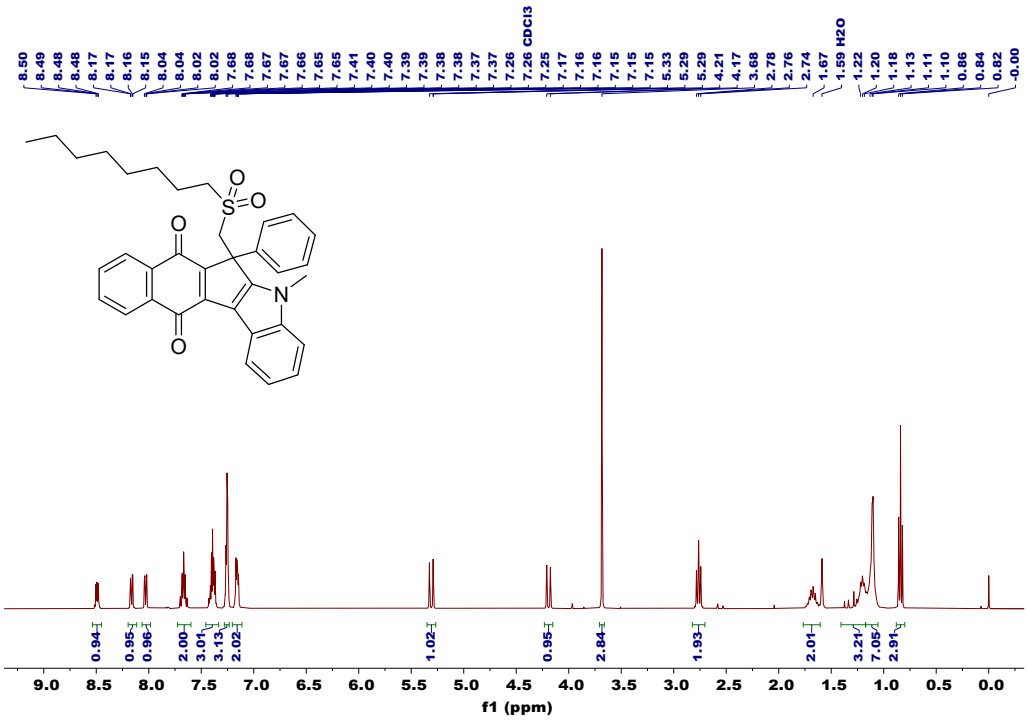


^{13}C {^{1}H} NMR (101 MHz)

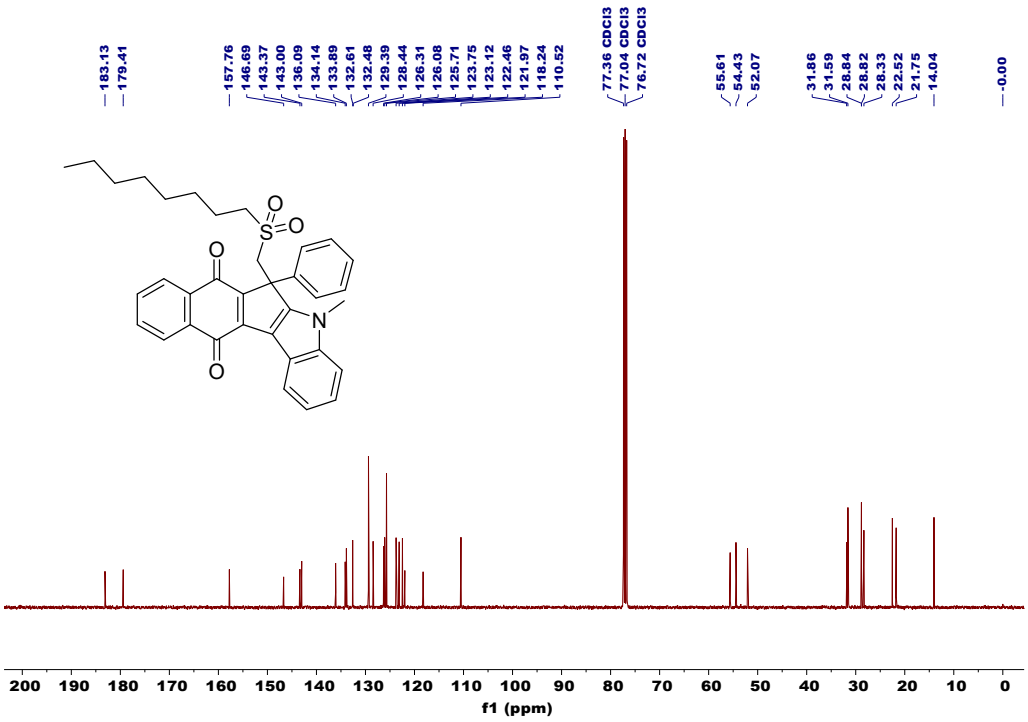


5-methyl-6-((octylsulfonyl)methyl)-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (29)

^{1}H NMR (400 MHz)

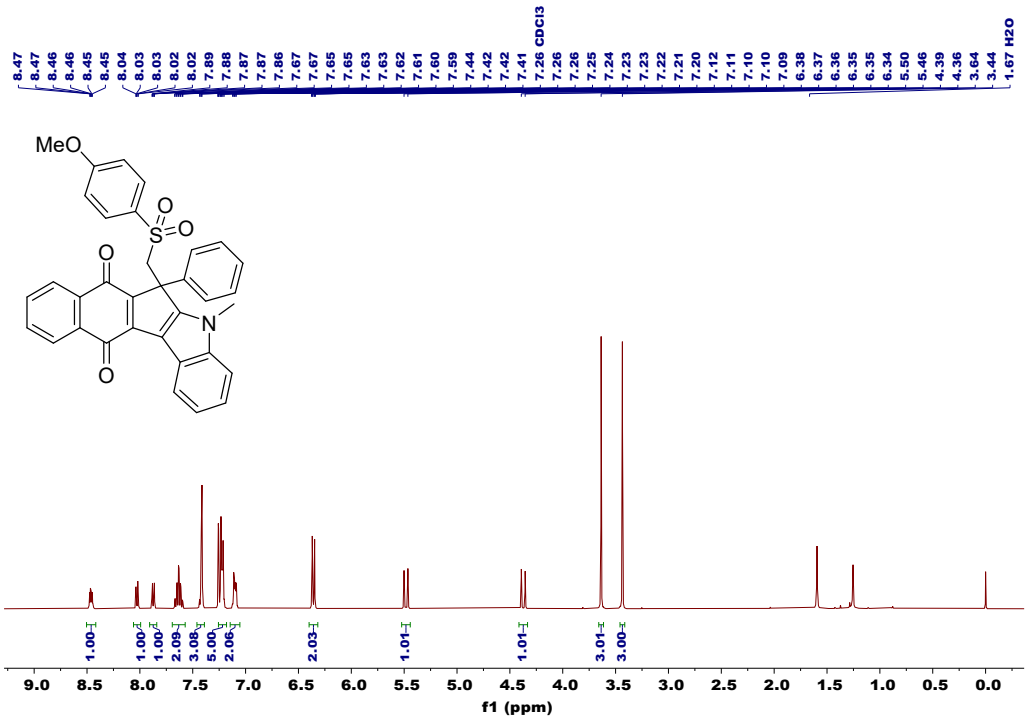


^{13}C {^{1}H} NMR (101 MHz)

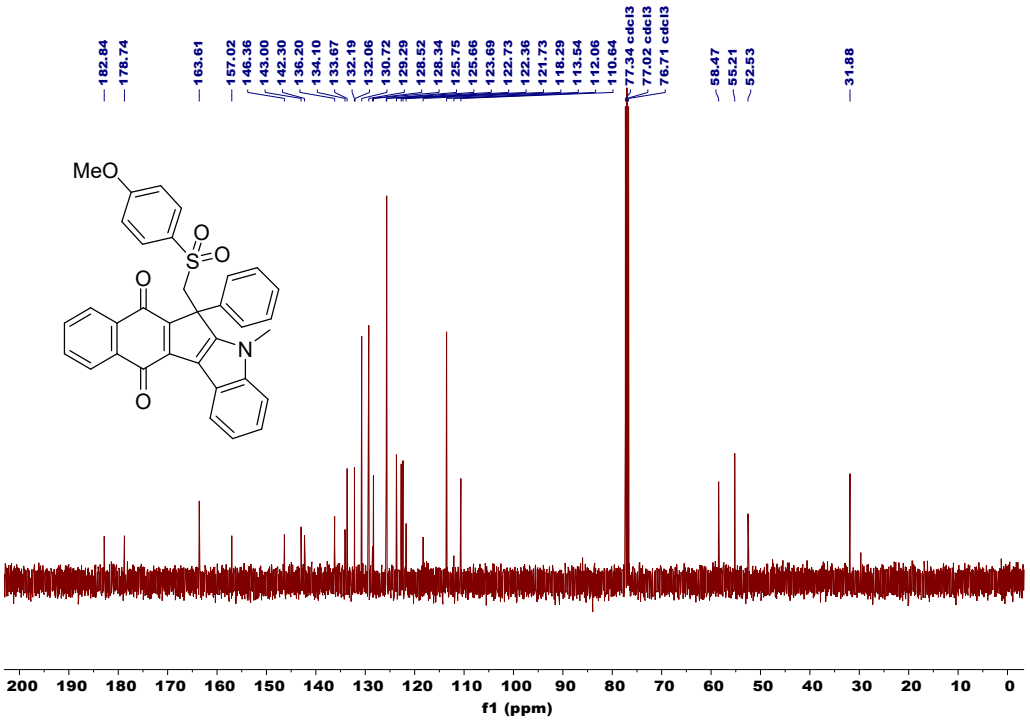


6-(((4-methoxyphenyl)sulfonyl)methyl)-5-methyl-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (30)

^{1}H NMR (400 MHz)

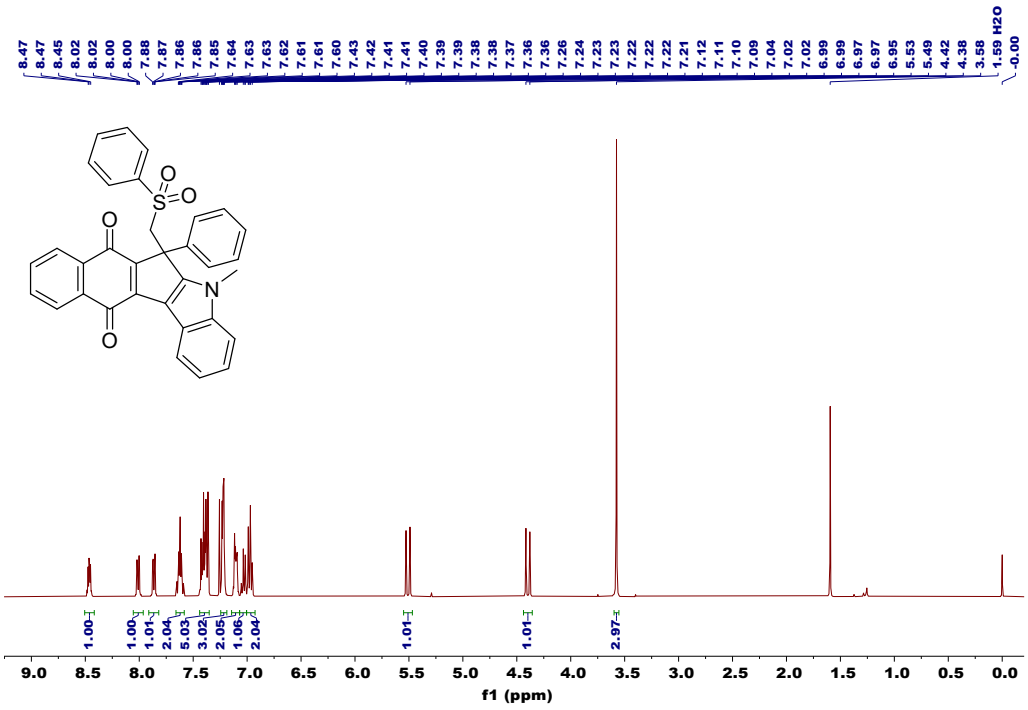


^{13}C {^{1}H} NMR (101 MHz)

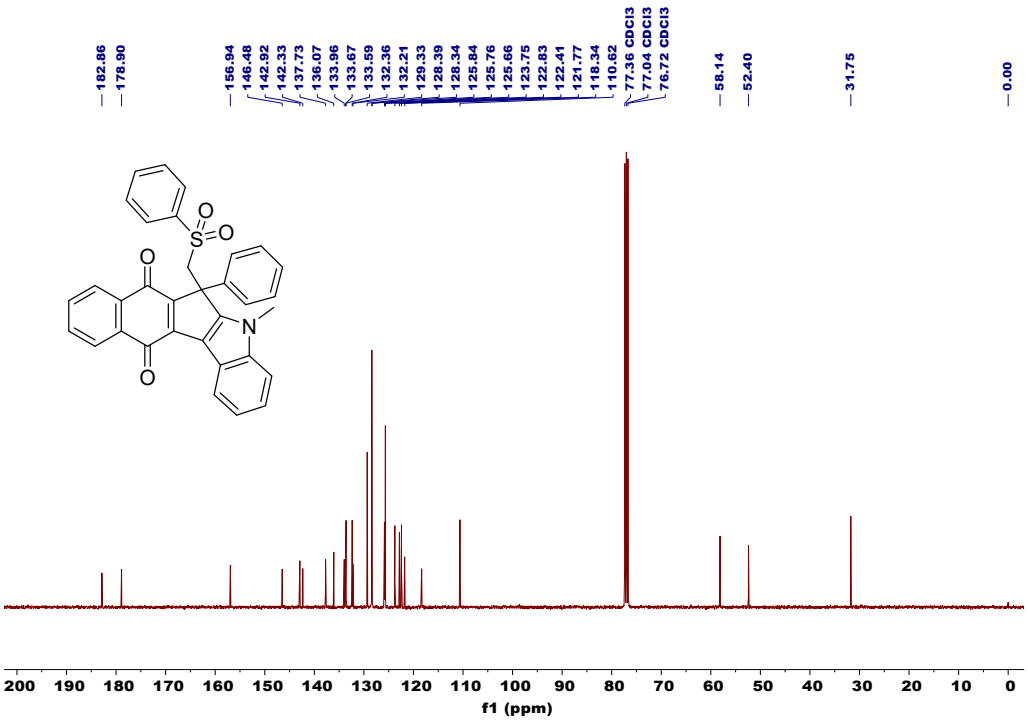


5-methyl-6-phenyl-6-((phenylsulfonyl)methyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (31)

^{1}H NMR (400 MHz)

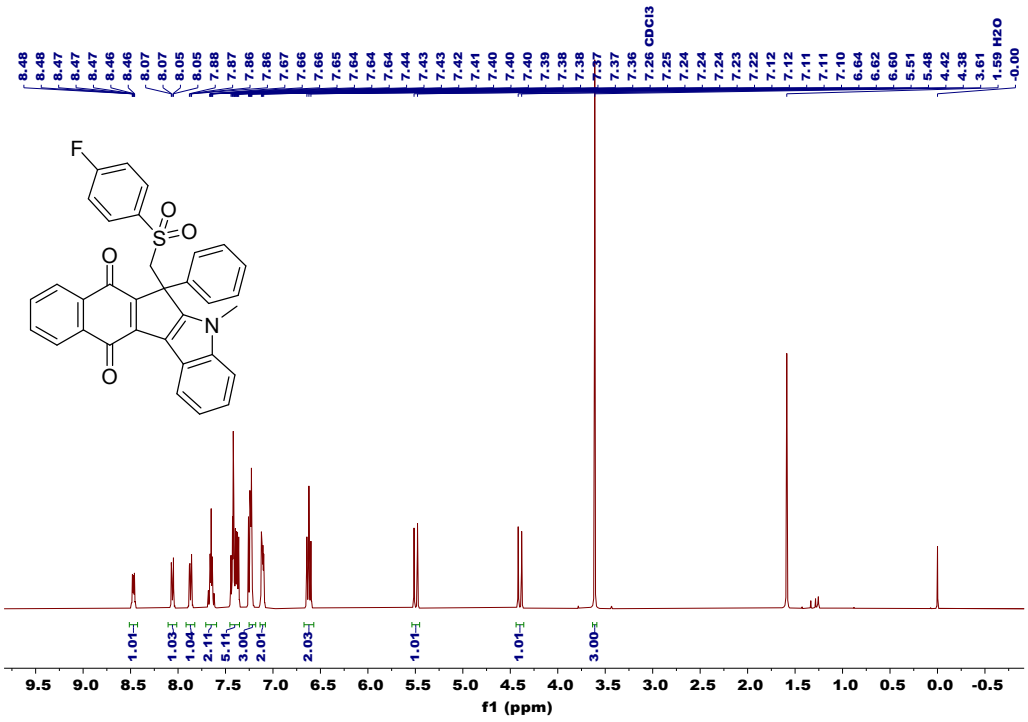


^{13}C {^{1}H} NMR (101 MHz)

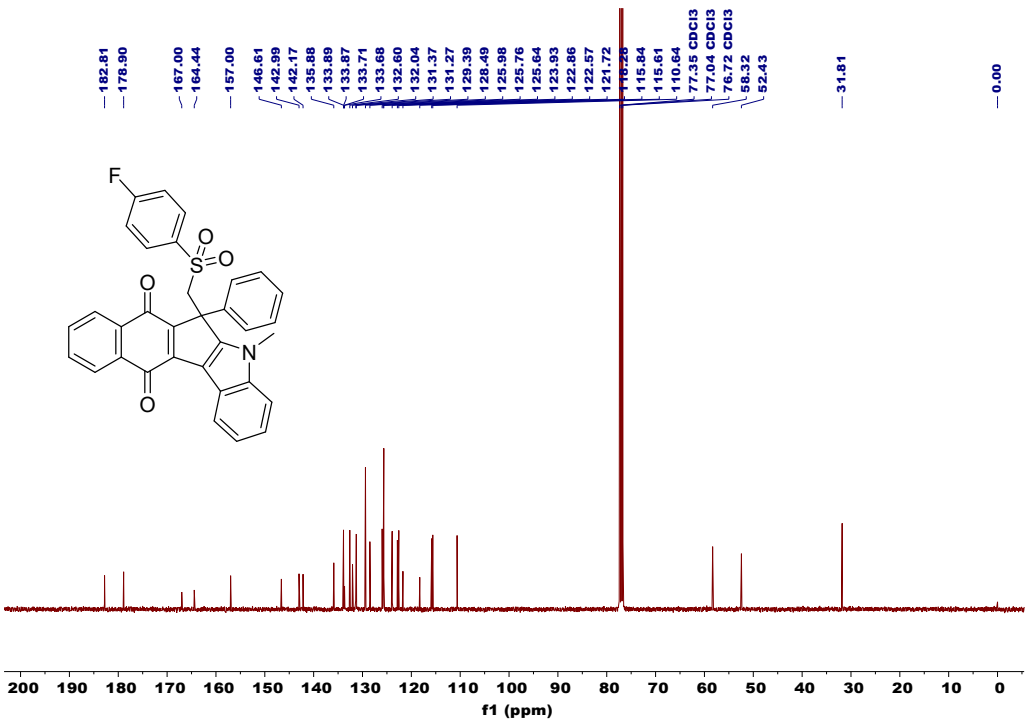


6-(((4-fluorophenyl)sulfonyl)methyl)-5-methyl-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (32)

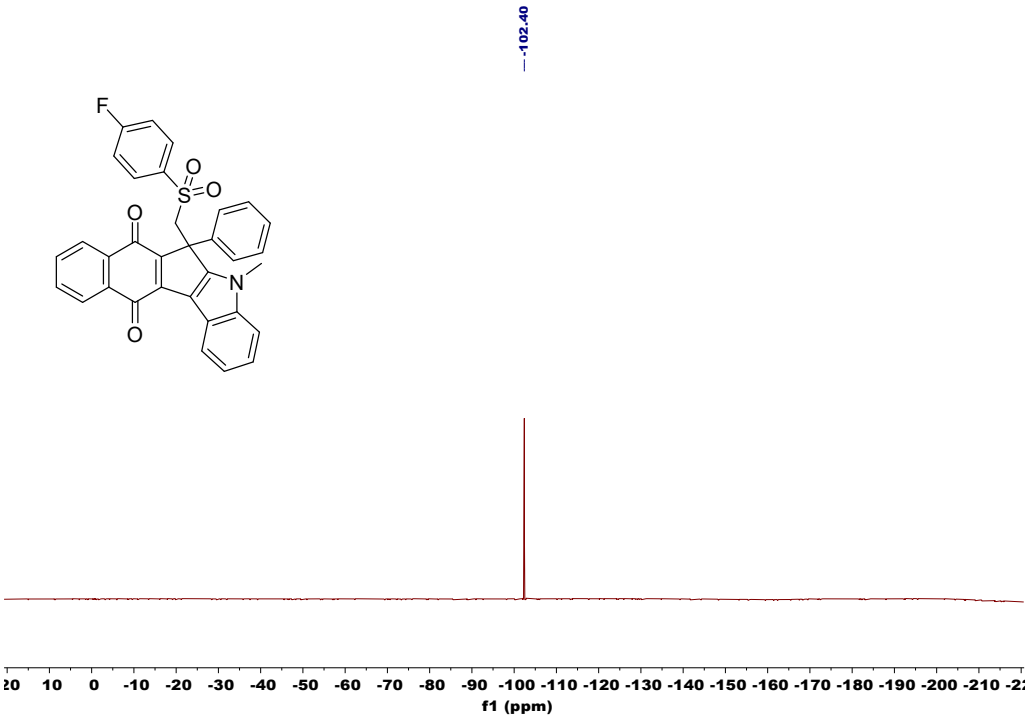
^{1}H NMR (400 MHz)



^{13}C {^{1}H} NMR (101 MHz)

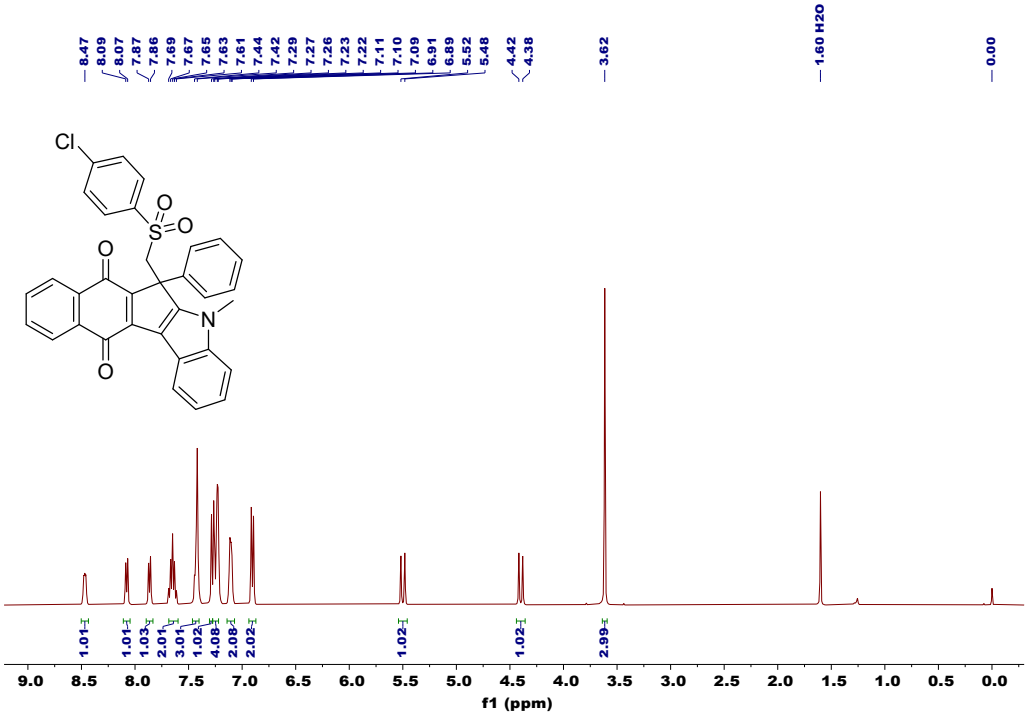


^{19}F {^{1}H} NMR (376 MHz)

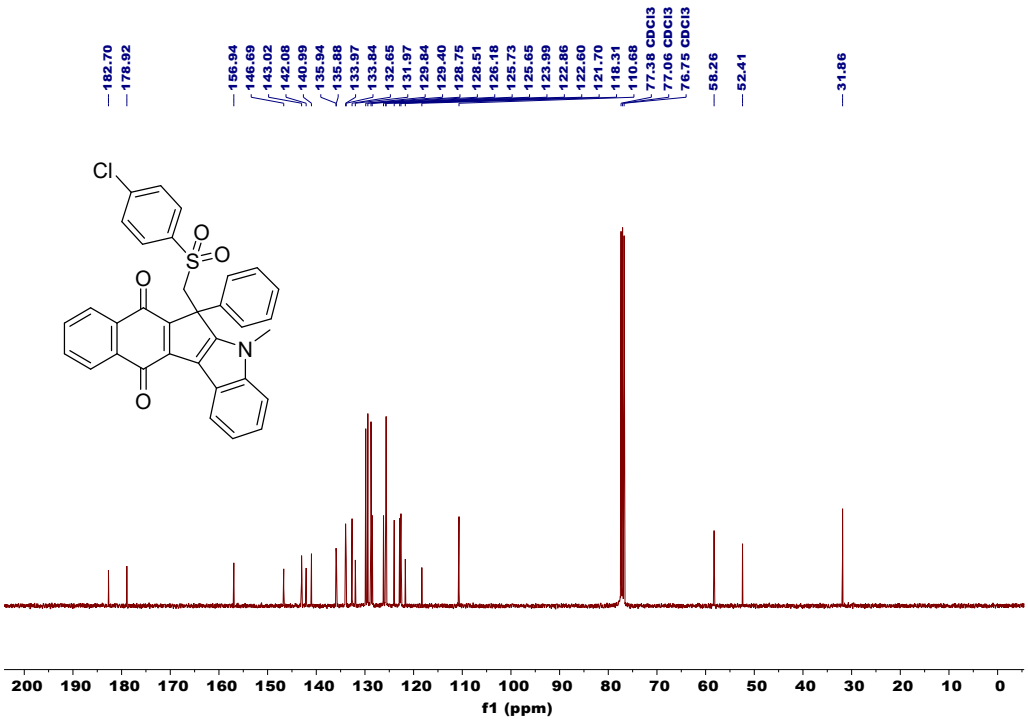


6-(((4-chlorophenyl)sulfonyl)methyl)-5-methyl-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (33)

^{1}H NMR (400 MHz)

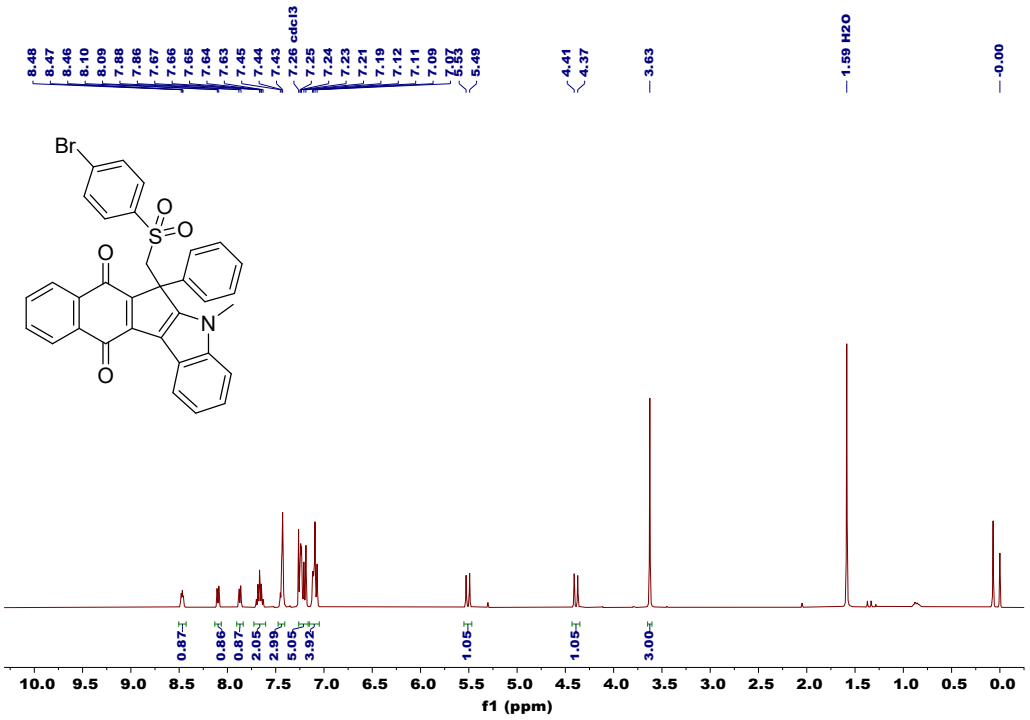


^{13}C {^{1}H} NMR (101 MHz)

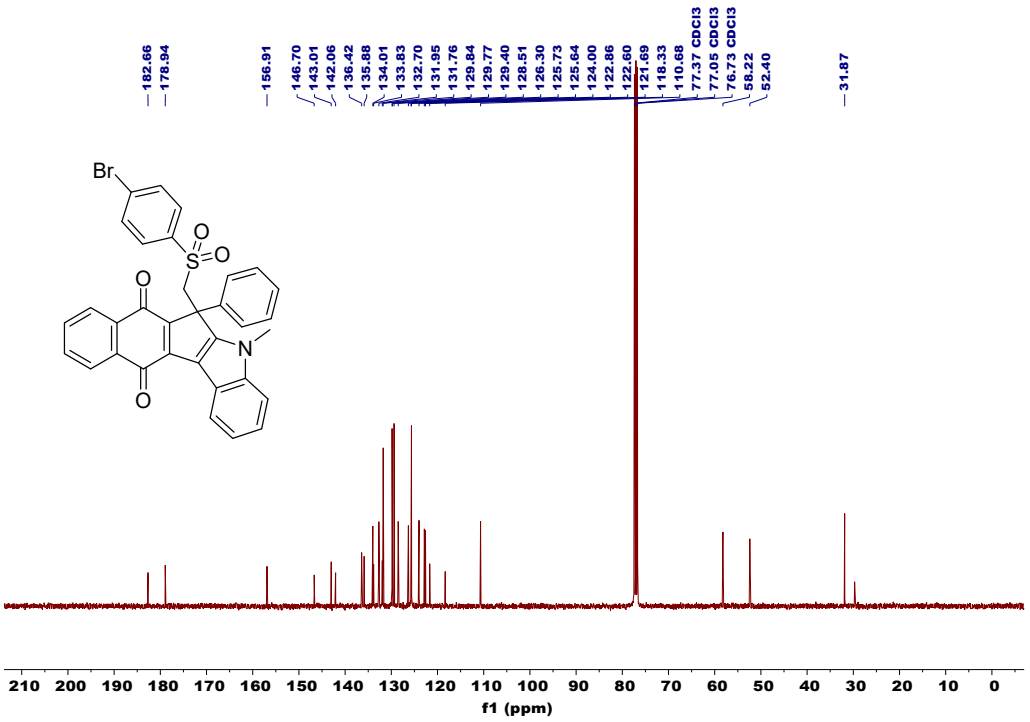


6-(((4-bromophenyl)sulfonyl)methyl)-5-methyl-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (34)

^{1}H NMR (400 MHz)

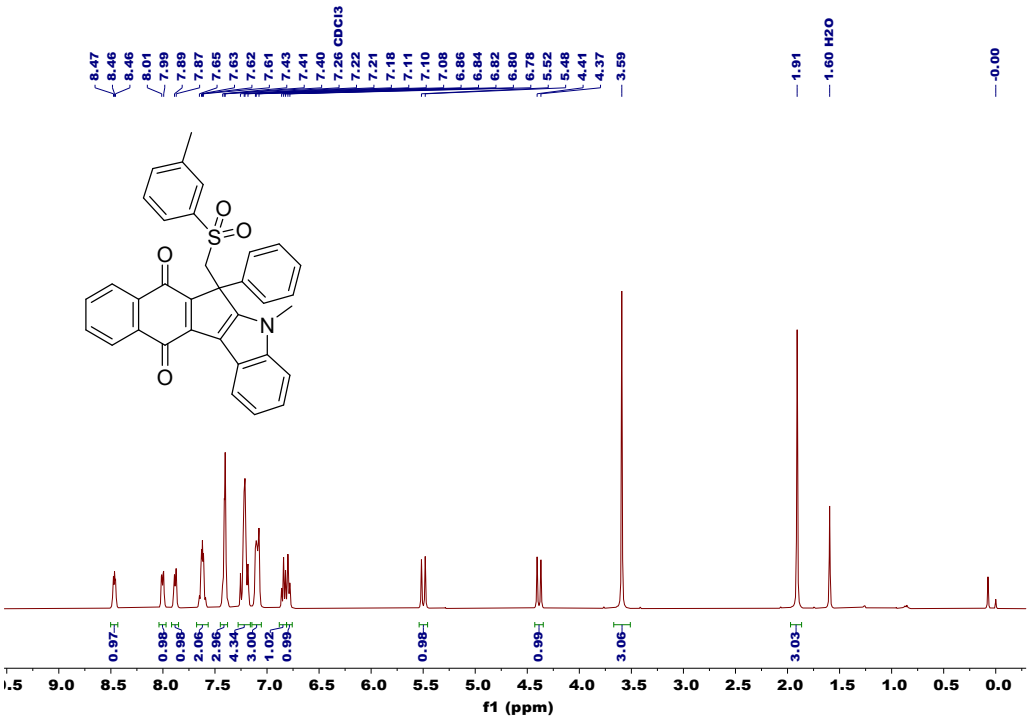


^{13}C {^{1}H} NMR (101 MHz)

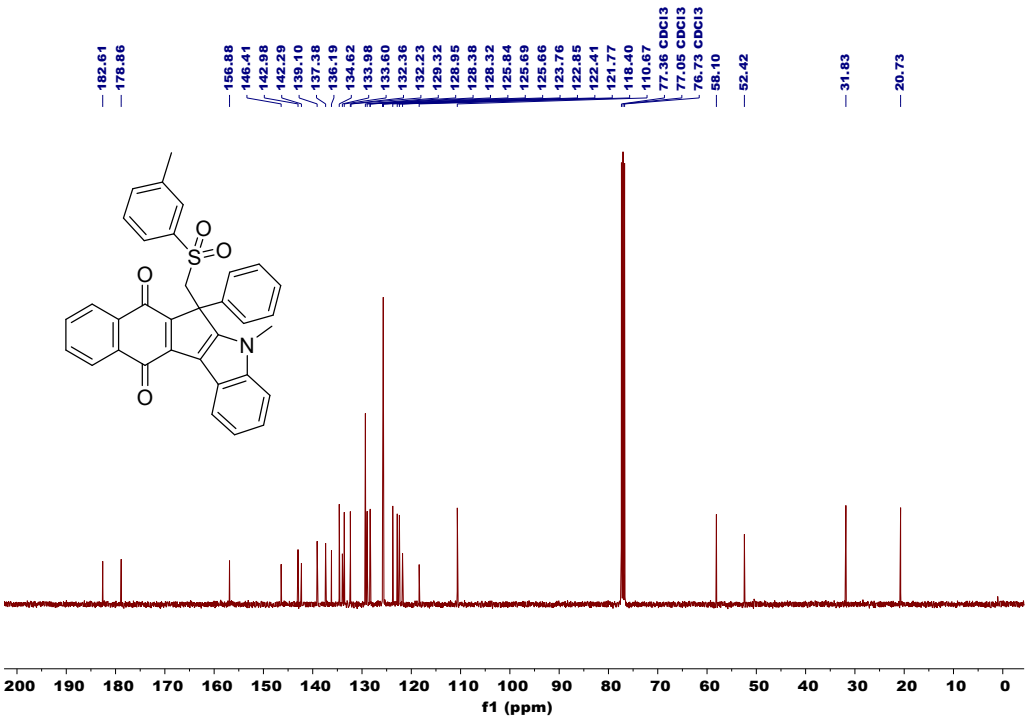


5-methyl-6-phenyl-6-((*m*-tolylsulfonyl)methyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (35)

^{1}H NMR (400 MHz)

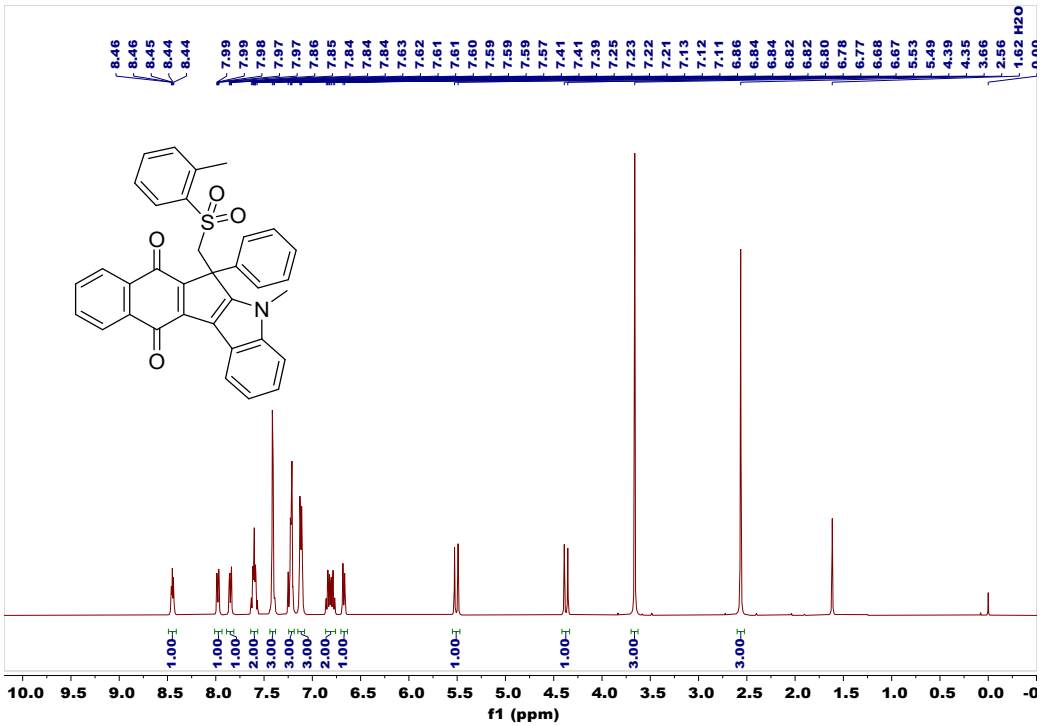


^{13}C {^{1}H} NMR (101 MHz)

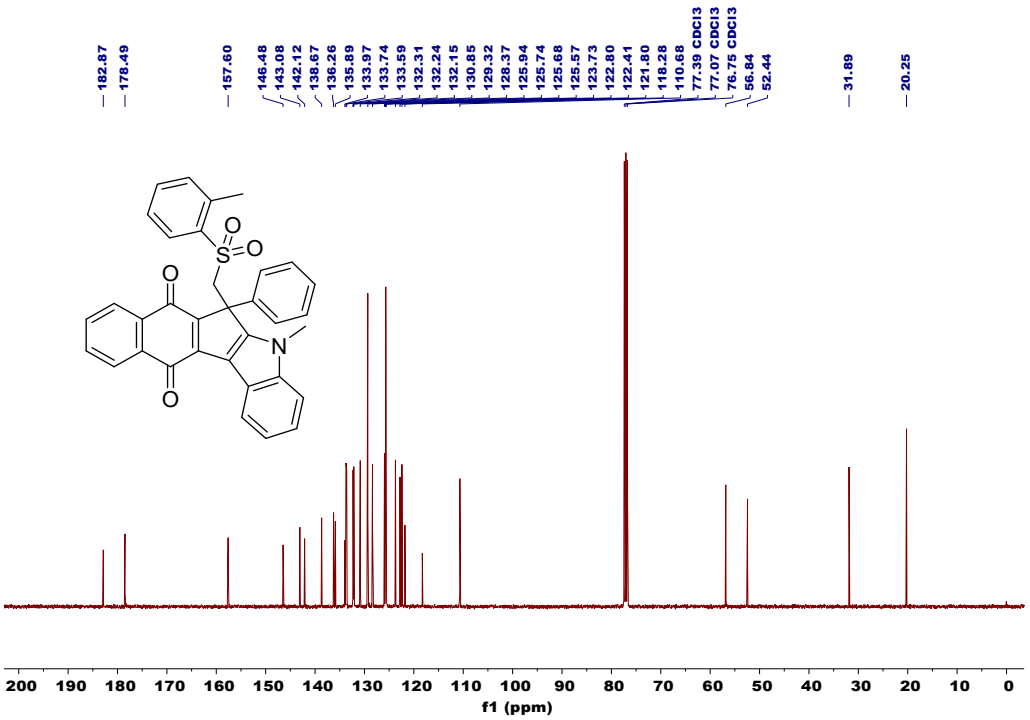


5-methyl-6-phenyl-6-((*o*-tolylsulfonyl)methyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (36)

^{1}H NMR (400 MHz)

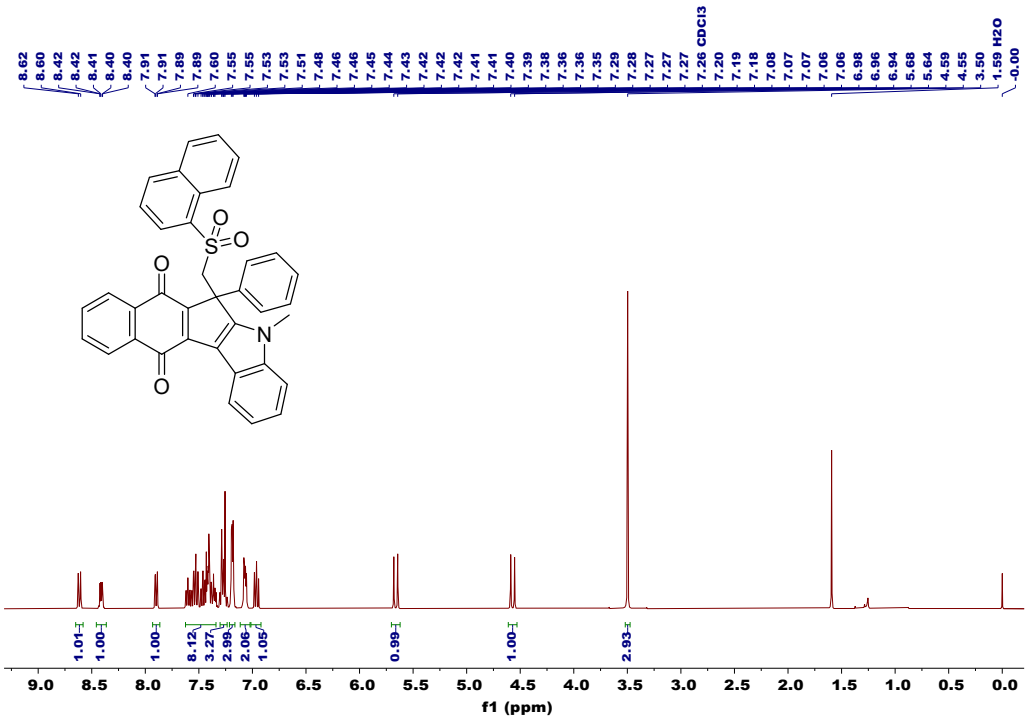


^{13}C {^{1}H} NMR (101 MHz)

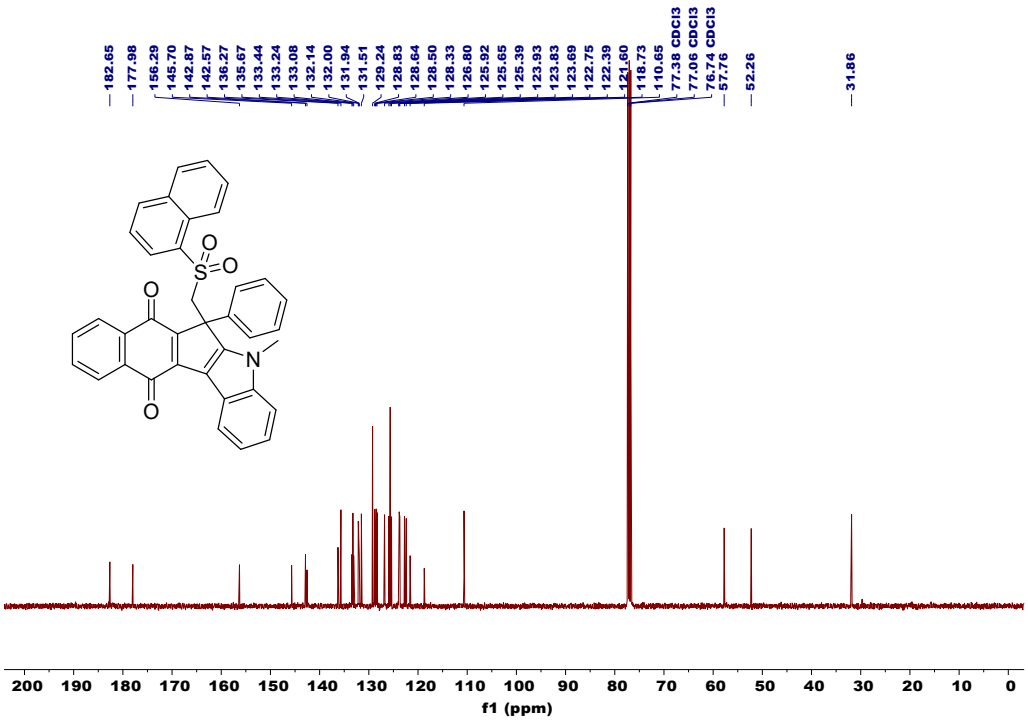


5-methyl-6-((naphthalen-1-ylsulfonyl)methyl)-6-phenyl-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (37)

^{1}H NMR (400 MHz)

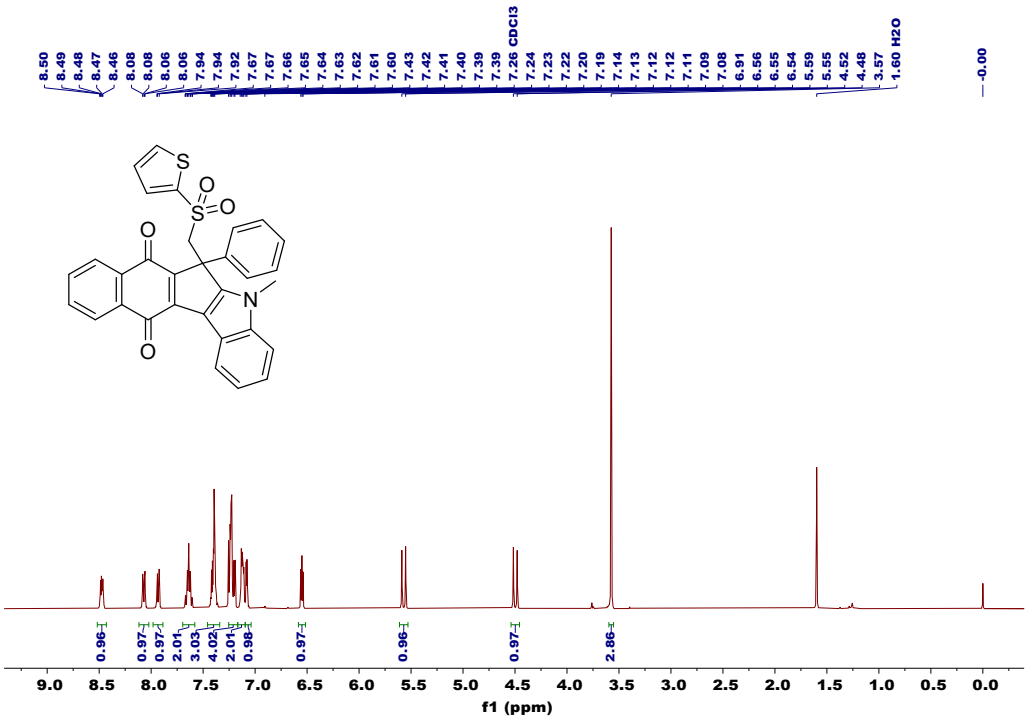


^{13}C {^{1}H} NMR (101 MHz)

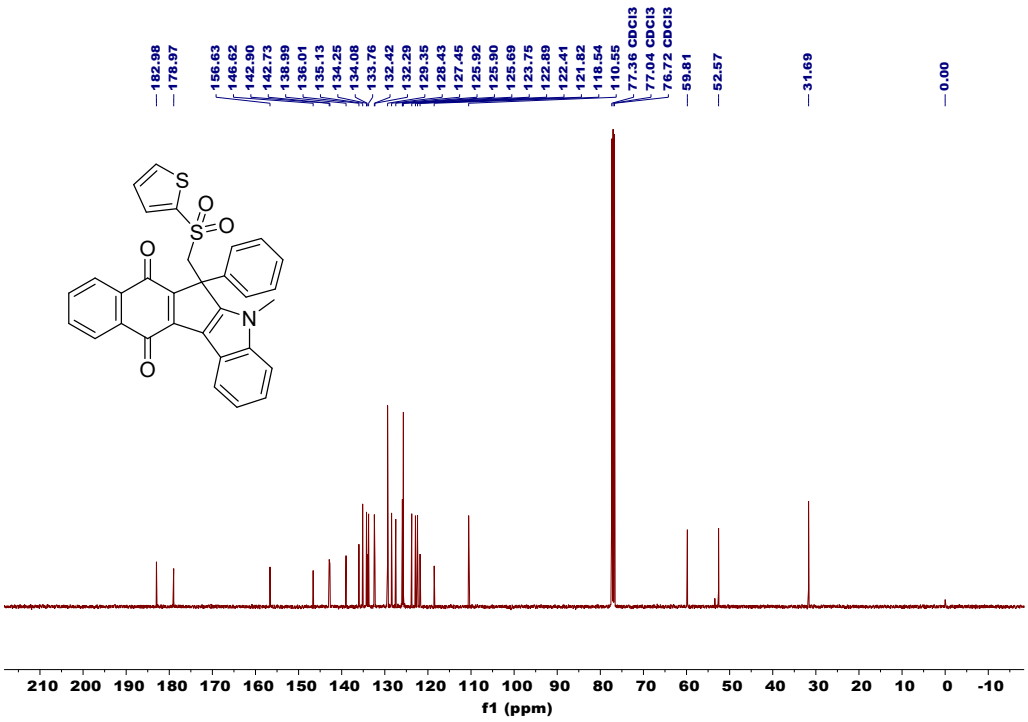


5-methyl-6-phenyl-6-((thiophen-2-ylsulfonyl)methyl)-5,6-dihydrobenzo[5,6]indeno[2,1-*b*]indole-7,12-dione (38)

^{1}H NMR (400 MHz)

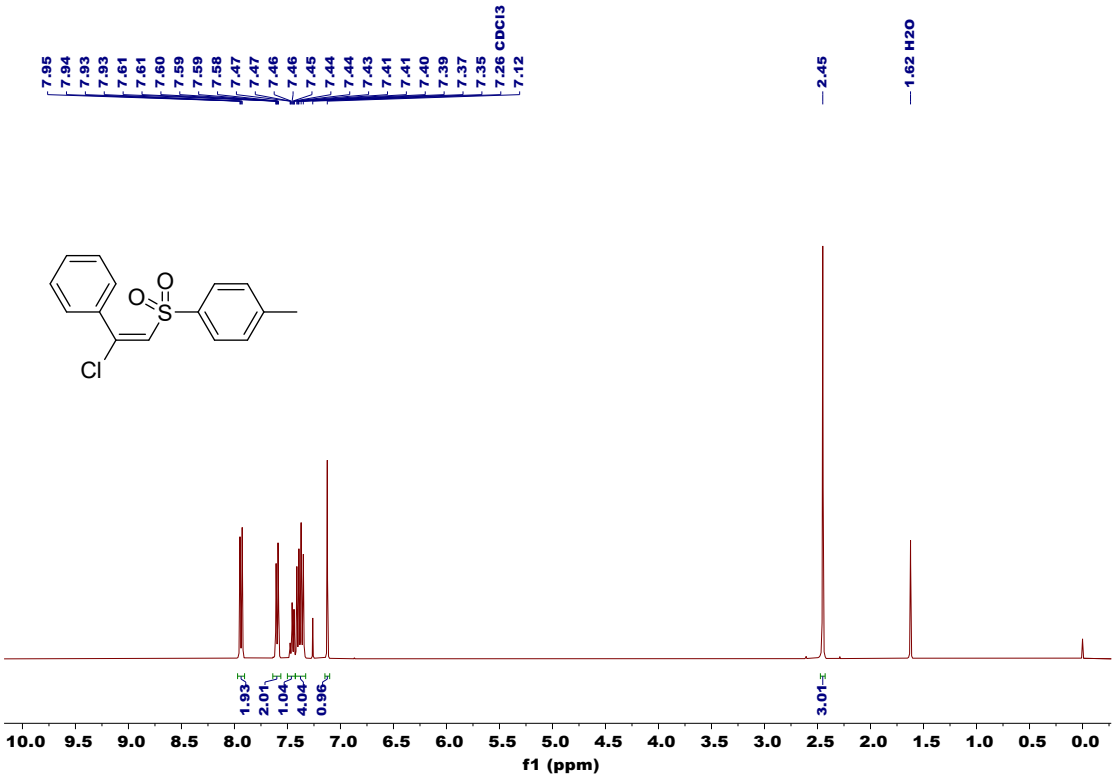


^{13}C {^{1}H} NMR (101 MHz)

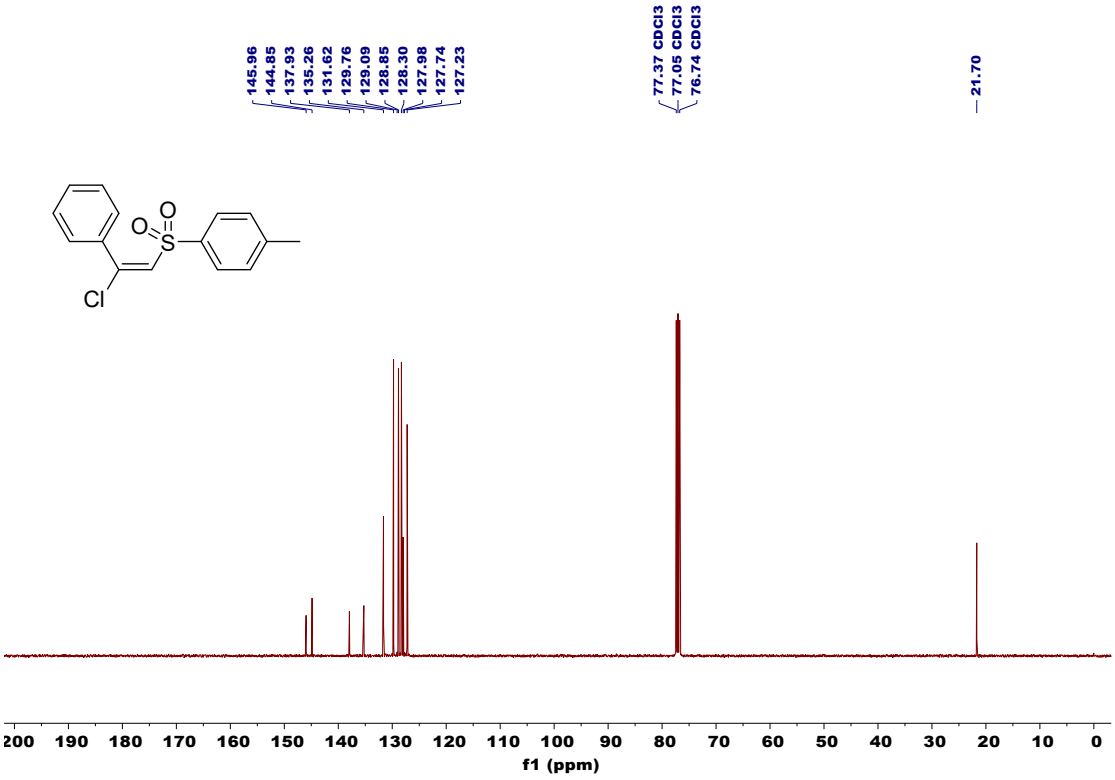


(*E*)-1-((2-chloro-2-phenylvinyl)sulfonyl)-4-methylbenzene (39)

^{1}H NMR (400 MHz)

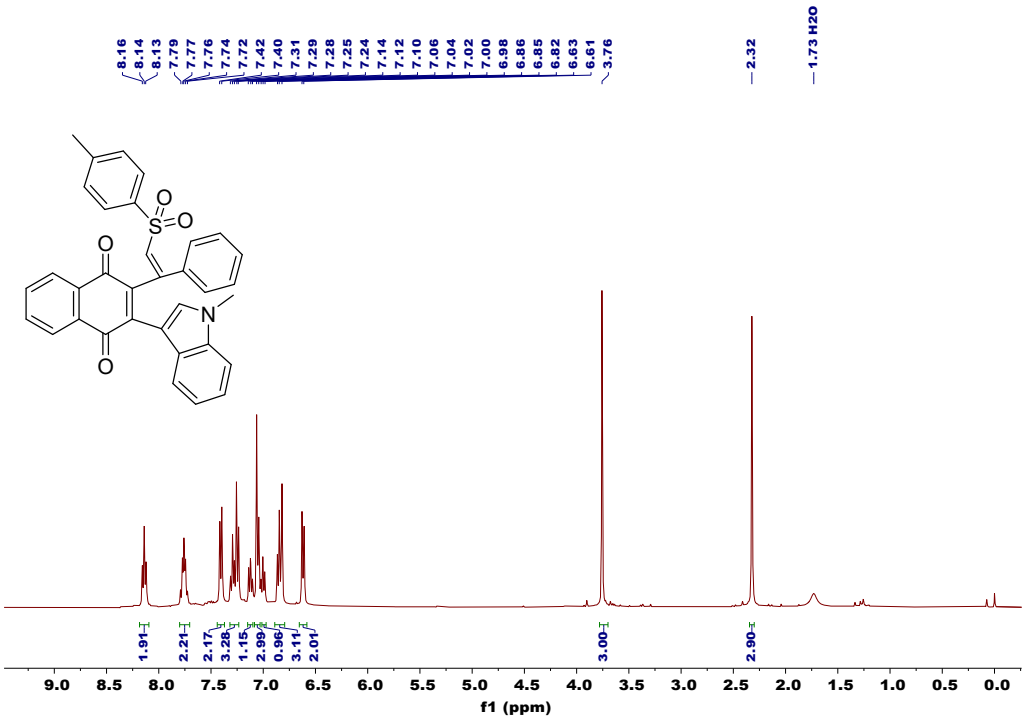


^{13}C {^{1}H} NMR (101 MHz)

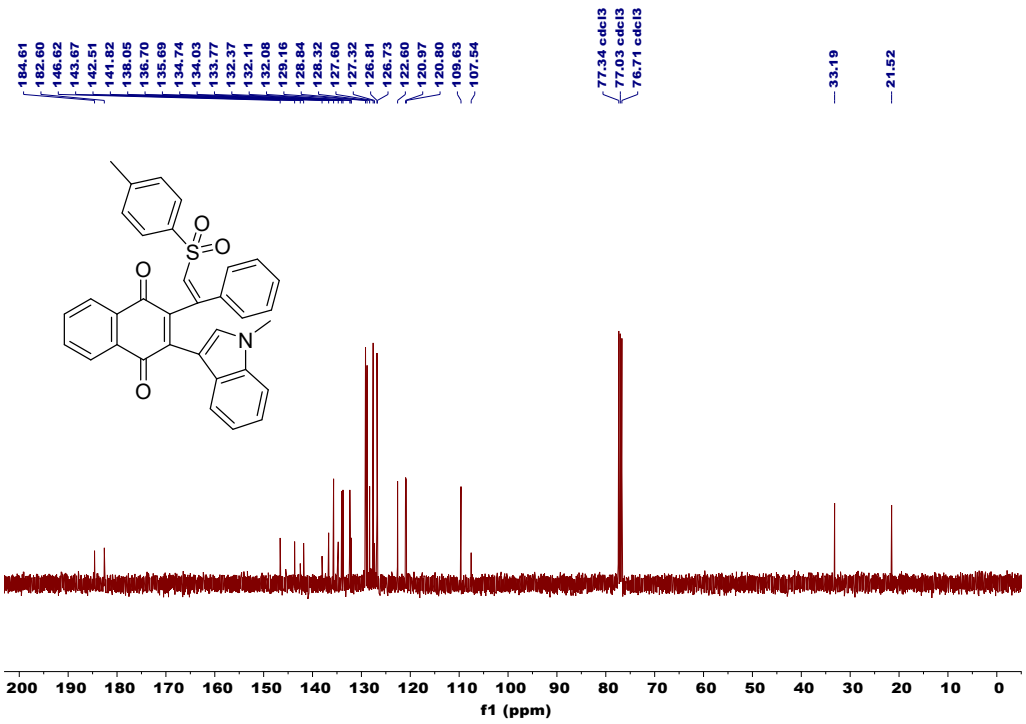


2-(1-methyl-1*H*-indol-3-yl)-3-(1-phenyl-2-tosylvinyl)naphthalene-1,4-dione (41)

^{1}H NMR (400 MHz)

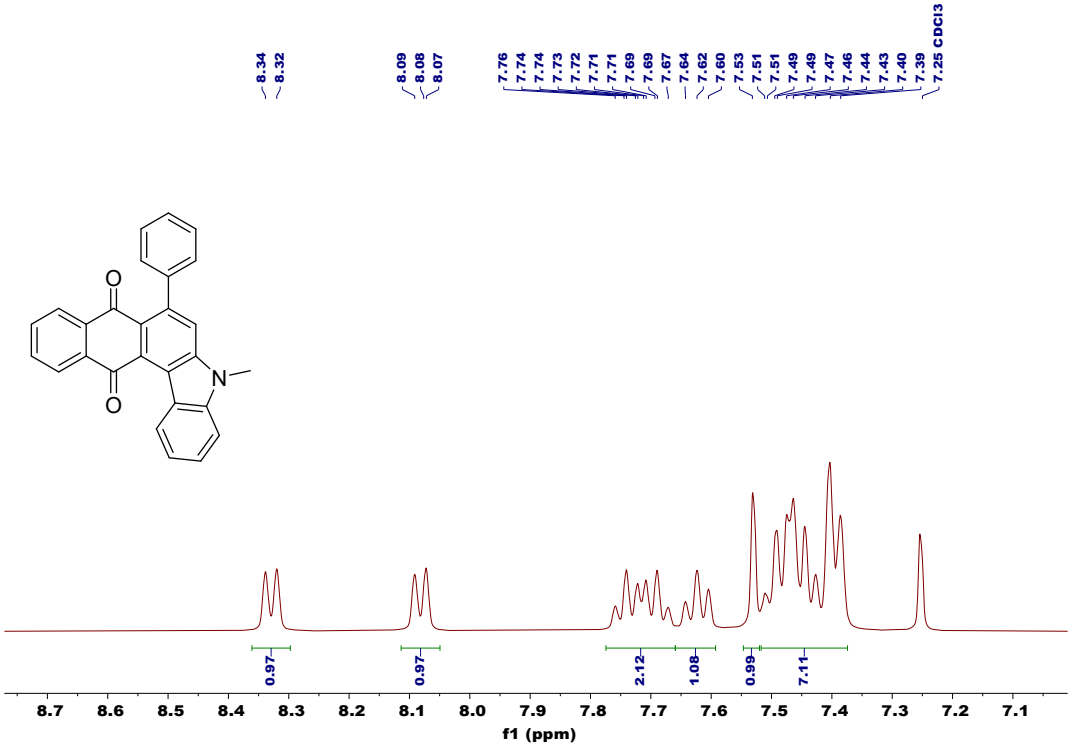


^{13}C {^{1}H} NMR (101 MHz)



5-methyl-7-phenyl-5H-naphtho[2,3-*c*]carbazole-8,13-dione (42)

^{1}H NMR (400 MHz)



^{13}C {^{1}H} NMR (101 MHz)